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AN X-RAY DIFFRACTION DATA REDUCTION PROGRAM FOR THE IBM 704 AND 7090

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PREFACE

This program is intended to provide a completely automatic process for reducing "raw" single-crystal x-ray diffraction intensity data to the form of structure factors. If desired, the data reduction may be extended to yield normalized structure factors. The program is applicable primarily to data obtained on film with Weissenberg and/or precession goniometers.

All programming has been done in IBM 704 FORTRAN II language. Binary program decks are available which are independent of any special operating system.

The printed output has been contrived to be easy to read and to give the program user easy access to all information necessary for further stages of the structure analysis. Also all information required for correction of the initial set of processed data are provided. The program detects some errors in intensity estimates and indexing, and indicates these both in a preliminary error-detection run and in the final output.

The magnetic tape output is consistent with the input of useful structure determination and refinement programs.

PROBLEM STATUS

This is an interim report; work on this problem is continuing.

AUTHORIZATION

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1. CAPABILITIES

Section 1 is intended to give a general impression of the capabilities of the program. Every effort has been made to make the program as general as possible, and it is felt that all contingencies within the intended scope of the program have been provided for.

1.1 Crystal Settings

Any number of crystal settings can be accommodated as long as the size of the problem remains within the limits given in section 2. The goniometer type, x-ray wavelength, and zone axis indices are specified for each setting. General settings may be used; e.g., a setting such as [11$\bar{2}$] may be specified as well as the common [100], [010], [001] settings.

1.2 Independently Observed Sets of Data

Any number of independently observed sets of data collected from a given crystal setting may be accommodated as long as the size of the problem remains within the limits given in section 2.

1.3 Intensity Data

The program accepts "raw" intensity data collected by multiple film Weissenberg or precession techniques. That is, as each intensity estimate is read, its value is recorded on a data sheet which will be given to a key punch operator without further manipulation by the crystallographer. The data are grouped for key punching, computer input, and processing into sets, each of which will consist of data read from a pack of films containing data from one reciprocal lattice layer.

The data from the different films in the multiple film packs are correlated and averaged. The correlation is done independently for each pair of adjacent films, and the averaging is done independently for each set of data.

Intensity estimates which give abnormal ratios of intensities (i.e., film factors) on adjacent films are rejected from further consideration in the processing unless normal ratios, involving a third or more films, also are found. Rejection or acceptance of each film factor is decided by comparison of each film factor with the average for the relevant pair of adjacent films. Acceptance criteria are specified by the program user for each crystal setting. The averaging and inspecting process is iterated until no further rejections occur. The procedure used is described further in section 3.2. Reflections lying outside the range of observation but mistakenly included in the observed set also are rejected. Rejected reflections are listed in a separate preliminary output especially designed for this purpose, and also are clearly labeled in the final data output.

More than one estimate of a given reflection may be included in any set. If these are to be averaged later (see section 1.6) they must be given identical Miller indices (e.g., the program does not recognize that $|F(hk\ell)| = |F(\bar{h}\bar{k}\bar{\ell})|$, see section 2.1).

Reflections with intensities too weak to be observed may be included. Reflections absent because of space group extinction should not be included.

The reflections within a set need not be arranged in any special order prior to loading into the computer. The data within each set are arranged in dictionary order of h, k, ℓ in the first phase of the calculation. However, if the data are arranged in dictionary order of h, k, ℓ prior to loading into the computer, the first part of the calculation may be omitted.

Within any independently observed set or "layer" of data, two different intensity scales may be used for estimating intensities. For example, one scale may cover the range of intense reflections while the other scale covers the range of weak reflections. The correlation factor relating the two scales must be known.

Any independently observed set of intensity data may be on a arbitrary scale which has not been correlated with any other set of data.

The data may be loaded into the computer from either punched cards or magnetic tape.

1.4 Lp and Spot Shape Corrections

The data are corrected for the Lorentz and polarization effects. For Weissenberg data correction may or may not be made for compaction or expansion of spot shapes on upper layer photographs. Where both expanded and compacted spots are estimated from the same films, the compacted data must be treated as a set separate from the expanded data. The method of Phillips (1) is used for this correction. Where possible, the expanded spots should be used because the correction factor for compacted spots passes through zero at low $(\sin\theta)/\lambda$. When the spot shape correction factor is equal to or less than 10^{-2}, the intensity for that reflection is set equal to zero and the reflection is listed with the rejected data.

The equations of Waser (2) are used for the precession Lp Corrections.

1.5 Absorption Corrections

The program does not calculate absorption corrections, but provision is made in the input for inclusion of previously determined absorption corrections. The corrections are applied automatically in the computer.

1.6 Correlation of Independently Observed Sets of Data

If more than one crystal setting has been used in collecting the data, the independently observed sets of data are correlated and put on a common arbitrary scale by the least squares procedure of Rollett and Sparks (3). The weighting of observations is done as follows: The relevant observations consist of pairs of nonzero intensities having identical sets of Miller indices, each intensity of a pair having been obtained from a different crystal setting. Each intensity of a pair is multiplied by the factor $(n_a + n_b)/(I_a + I_b)$, where the subscripts a and b identify the individuals of the pair, n is the number of films from which the intensity has been estimated, and I is the value of the intensity estimate corrected for Lp and spot shape. The reflection data must be arranged in dictionary order of h, k, ℓ at this point in the calculation. The eigenvalue-eigenvector solution is obtained by a

modified version of SHARE program AN F 202 (distribution number 664) and SHARE program RW VCTR (distribution number 635). These programs are FORTRAN coded.

1.7 Final Averaging of Data

After having been scaled to a common basis, all equivalent data (i.e., all data with identical Miller index triples) are averaged and the data are arranged in a single listing in dictionary order of h, k, ℓ. In computing average intensities, the individual intensities are weighted according to the number of films from which each was estimated. The data also are maintained in unaveraged form in the sets or "layers" as originally observed.

1.8 Placing the Data on the Absolute Scale

The data are placed on the absolute scale by means of a modified Wilson function suggested by Schoomer and Hauptman (4). The function used is

$$\log K_i = A + BS_i^X$$

where A, B, and X are constants determined as described below, S_i is the value of $(\sin\theta)^2/\lambda^2$ at the middle of the ith increment in $(\sin\theta)^2/\lambda^2$ within which values of K_i are calculated, and

$$K_i = \frac{\sigma_i \, \Sigma\, \epsilon}{\Sigma\, I}$$

where ϵ is the integer factor used to convert E^2 (the normalized structure factor (5)) to $\mathcal{E}^2$ (the quasi-normalized structure factor (6)), I is the F^2 value on an arbitrary scale, and $\sigma_i = \sum_i^N f_i^2$. The summations are taken over all reflections observed in the ith increment of $(\sin\theta)^2/\lambda^2$.

The constants A and B are found by calculating least squares fits for values of X ranging from 1 through 10 in increments of 0.5. The "best parameters" are those yielding the smallest sum of squares of residuals. In the least squares calculations each observation is weighted according to the number of reflections contributing to it.

A fixed increment in $(\sin\theta)^2/\lambda^2$ is used in the calculations. This increment is specified by the program user. The range of the function is to the edge of the sphere of reflection implied by the smallest wavelength used. Reflection data need not be observed in all increments in this range.

The atomic scattering factors f are calculated using the equation

$$f = A\exp[-a(\sin\theta)^2/\lambda^2] + B\exp[-b(\sin\theta)^2/\lambda^2] + C$$

proposed by Vand, Eiland, and Pepinsky (7). Values of the constants A, a, B, b, and C have been calculated and tabulated for a large number of atoms and ions by Forsyth and Wells (8). The approximations are good through the molybdenum range of $(\sin\theta)/\lambda$.

1.9 Preliminary Output

The preliminary output occurs during the phase of the calculation consisting of film-to-film averaging of intensity data and correction for Lp and spot shape effects. This

output may be observed in a pilot run for the purpose of error detection. In this case, the data do not need to be arranged in dictionary order of h, k, ℓ, and the first part of the calculation, DICNRY, may be omitted. The data processing may be stopped by sense switch control after completion of the preliminary output. This output consists of:

A. The film factors for each independent set of data (see section 1.3). These are printed immediately after the Lp corrections have been applied and before the next set of data are read into the computer. The output for each layer or set of data consists of:

1. the zone axis indices, U, V, W
2. the layer number, LN
3. the number of reflections in the set, NR
4. the five film factors.

B. Rejected reflections are listed, along with sufficient information to identify their original sets, after all of the data have been processed as far as application of the Lp corrections. The output for each layer or set of data consists of:

1. U, V, W
2. LN.

The output for each rejected reflection is:

1. h, k, ℓ
2. $(\sin\theta)^2/\lambda^2$
3. the square root of the Lp correction factor (including the spot shape correction factor)
4. $|F|^2$
5. A column headed with R in which rejections are indicated as follows:

a. A 1 indicates that the rejection is a result of an abnormal film factor.

b. A 10 indicates, for Weissenberg data, that the reflection lies outside the sphere of reflection implied by the x-ray wavelength specified for the relevant crystal setting. For precession data, a 10 indicates that the reflection lies beyond the range of accessibility of the goniometer for the particular settings specified.

c. A 20 indicates that the spot shape correction factor is equal to or less than 10^{-2}. This type of rejection can occur only for compacted reflections observed on upper layer Weissenberg photographs.

The rejection numbers are additive. Thus an 11 would indicate that the reflection datum suffers from both an anomalous film factor and incorrect indexing. A 20 could possibly indicate that the relfection has been observed twice with incorrect indexing, etc. In any case, the unaveraged data listed in the sets, as originally observed (see section 1.10.C) should be consulted to determine the exact nature and location of the difficulty.

The preliminary output may be observed on-line if so desired. In any case, it is written on the BCD output tape for off-line printing.

1.10 Output of Structure Factor Data

The BCD output of structure factor data for off-line printing may be divided into three classifications, A, B, C, as follows:

A. The data are listed in dictionary order of h, k, ℓ. All $|F|^2$ data with equivalent h, k, ℓ are averaged in this output (see section 1.7). Each independent reflection is listed only once. The output for each reflection is:

1. h, k, ℓ
2. $(\sin\theta)/\lambda$
3. $|F|^2$
4. $|F|$
5. ϵ, i.e., the integer factor required to convert E^2 to $\mathcal{E}^2$.
6. The total number of films from which nonzero estimates of the intensity were made. This column is headed W, and these quantities will be hereafter designated by W.

Following the last reflection in this listing is the total number, modulo 32728, of independent data printed (including rejected data).

B. The modified Wilson equation parameters and sufficient data to hand-plot the "K curve" – specifically:

1. A, B, X from the equation

$$\text{Log } K = A + B\,[(\sin\theta)^2/\lambda^2]^X.$$

2. The "absolute base" scale factor determined from A, i.e., the factor by which the correlated $|F|^2$ data are to be multiplied to put them on the absolute scale.
3. Midincrement values of $(\sin\theta)^2/\lambda^2$.
4. The observed values of log K (Naperian base).
5. The numbers of reflections observed within each increment of $(\sin\theta)^2/\lambda^2$.

C. Finally, the data are listed in the sets or "layers" of independently observed data as they were fed into the computer. These data have not been averaged with other equivalent data. The data within each set are listed in dictionary order of h, k, ℓ. At the head of each set are the zone indices [UVW], the layer number, the printed words PRECESSION or WEISSENBERG to identify the goniometer type, the number of data in the set, and a scale factor which is the product of the layer least squares correlation factor and the "absolute base" scale factor determined from the modified Wilson function. The output for each reflection is:

1. h, k, ℓ
2. $(\sin\theta)/\lambda$
3. The square root of the Lp factor (including the spot shape correction factor if this has been applied).
4. $|F|^2$
5. $|F|$
6. ϵ

7. W and R as explained previously except that these quantities now are applicable to the individual sets of data only (see sections 1.10.A and 1.9.B).

In addition to the printed output, two BCD tapes are written in a format consistent with the least squares refinement program of Busing and Levy (9). These tapes contain:

Tape 5 – The averaged data in the form of h, k, ℓ, $|F|^2$, a least squares weighting factor which is equal to $|F|/\sqrt{W}$, where W is defined above (section 1.10.A), and $(\sin\theta)/\lambda$ (in columns 55-63 to be stored in T13 (9)). The data are listed in the same order as in the printed output.

Tape 7 – The same information for the unaveraged independent sets of data. The data are listed in the same order as in the printed output.

1.11 Normalization of the Structure Factors

If so desired, the data reduction may be extended to yield functions of $|E|$. The conversion from $|F|$ values to $|E|$ values is done as follows: The $|F|^2$ data are corrected for the temperature effect using the analytical expression for the K curve as implied by the equations in section 1.8. The resulting $|F|^2$ values are then divided by $\epsilon \sum^N f_i^2$. The values of f are calculated as described in section 1.8.

1.12 Output of Normalized Structure Factor Data

The printed output is quite similar to the printed output of F data already described. It is divided into three parts, A, B, and C, as follows:

A. The averaged data are listed in dictionary order of h, k, ℓ. Each independent reflection is listed only once. The output for each reflection is:

1. h, k, ℓ
2. $(\sin\theta)/\lambda$
3. $|E|^2 - 1$
4. $|E|$
5. ϵ, W, and R as defined previously (see section 1.10.A).

B. The "K curve" parameters and average values for several functions of $|E|$.* Specifically:

1. A, B, X from the equation $\text{Log}\,K = A + B[(\sin\theta)^2/\lambda^2]^X$
2. The "absolute base" scale factor determined from A.
3. $\langle|E|\rangle$
4. $\langle||E|^2 - 1|\rangle$
5. $\langle|E|^2 - 1\rangle$

C. Finally, the data are listed in the sets or "layers" of independently observed data as they were fed into the computer. The data within each set are listed in dictionary order of h, k, ℓ. These data have not been averaged with other equivalent data. At the head of

*The program does not take cognizance of the fact that for structures giving rise to both real and complex structure factors the averages for the corresponding sets of intensities are different. Usually, the proportion of real structure factors is small and this factor may be ignored; however, occasionally it will have to be taken into account.

each set are the zone indices [UVW], the layer number, the printed words PRECESSION or WEISSENBERG to identify the goniometer type, and the number of reflections in the set. The output for each reflection is:

1. h, k, ℓ
2. $(\sin \theta)/\lambda$
3. A factor K by which the $|F|^2$ values, already scaled on the absolute base, are to be multiplied to convert them to $|E|^2$ values.
4. $|E|^2 - 1$
5. $|E|$
6. ϵ, W, R as defined previously (see section 1.10.A).

In addition to the printed output, two BCD tapes are written in the format of the Fourier program of Sly and Shoemaker (10). These tapes contain:

Tape 5 – The averaged data, listed in the same order as in the printed output, in the form of h, k, ℓ and $|E|^2 - 1$.

Tape 7 – The same information written on tape for the unaveraged independent sets of data in the same order as in the printed output.

1.13 Ordering of $|E|$ and $|E|^2 - 1$ Data

If so desired, the data reduction may be extended to an arranging and output of the data in decreasing order of magnitude of $|E|^2 - 1$. These data are then segregated into groups specified according to evenness (g) or oddness (u) of h, k, and ℓ. Only data for which $|E|^2 - 1 \geqslant 0$ are listed.

The output consists of the following groupings:

1. All data	4. gug data	7. ugu data
2. ggg data	5. ggu data	8. guu data
3. ugg data	6. uug data	9. uuu data.

In all groups, the data are listed in decreasing order of magnitude of $|E|^2 - 1$.

1.14 Time of Computation

No formulas for estimating computing time are available. However, the following examples should suffice to give a general impression. The times given include time used in card program read-in and tape changes between the different parts of the calculations. The data were processed completely, from DICNRY through E ORDER.

Crystal	Settings	Sets	Input Reflections	Time	Computer
Cyclohexaglycyl	1	1	407	20 min	704
6-Hydroxycrinamine	2	11	4195	90 min	704
6-Hydroxycrinamine	2	11	4195	30 min	7090

2. LIMITATIONS

2.1 Indexing of Reflection Data

Care must be taken to maintain consistency in the assignment of Miller indices. The computer receives no crystallographic symmetry information. Therefore, crystallographically equivalent reflections must be assigned identical index triples to assure proper operation of the layer correlation and final intensity averaging calculations. Furthermore, the Miller index assignments must be consistent with the zone axis indices in a certain manner. The criterion of consistency is that

$$hU + kV + \ell W \geq 0$$

where h, k, ℓ are the Miller indices, and U, V, W are the zone axis indices for the relevant crystal setting.

2.2 Data Reduction to Structure Factor Form

1. The processing is limited to data collected by goniometers having the Weissenberg or precession geometries. Though primarily designed for processing film data, it will accommodate counter data obtained with Weissenberg or precession goniometers (e.g., the Geiger counter goniometer described by Evans (11)).

2. The program does not provide for calculation of absorption corrections. However, previously determined absorption corrections may be included in the input data for each reflection, and these corrections are automatically applied.

3. The number of different atomic species in the crystal must not exceed 20.

4. No more than ten different x-radiation wavelengths can be used in obtaining the data.

5. Number of data: Each independent set or "layer" of data may contain as many as 1000 reflections. Sets containing more than 1000 reflections may be divided into smaller sets of 1000 or less reflections. There may be as many as 50 sets of data. In total, the program will accommodate as many as 50,000 reflections involving as many as 300,000 intensity estimates.

6. The number of films from which any set of intensities has been estimated cannot exceed six.

7. If there is more than one crystal setting, each set of data must contain at least one nonzero reflection which also is observed with nonzero value from another crystal setting. The number of input reflections (as distinct from unique reflections) in common between two reciprocal lattice nets from different settings must not exceed 100 for each net.*

8. When one or several sets of data obviously are off-scale from the bulk of the data by as much as two or more orders of magnitude (as could happen when very short exposures are correlated with very long exposures) a preliminary scaling, sufficient to scale the data to roughly the same order of magnitude, is advisable. This may be done very conveniently by including the scale factor in the absorption correction factor.

*When a crystal setting is repeated in the input, as would happen when one or several layers are observed with both Weissenberg and precession goniometers, cross-correlation of these particular layers is not attempted by the program. However, all other correlation data involving these layers is used in the usual manner.

9. The total number of input reflections having the same Miller index h in common must not exceed 1000. The total number of input reflections having both h and k in common must not exceed 100.

10. The exponent X in the modified Wilson equation

$$\log K = A + B\,[(\sin\theta)^2/\lambda^2]^X$$

is restricted to integral and half integral values between 1 and 10 inclusive.

11. In evaluating the parameters A, B, and X in the modified Wilson equation, the number of intervals in $(\sin\theta)^2/\lambda^2$, within each of which K is evaluated from the experimental data, must not exceed 100.

12. Data obtained with radiation of wavelength shorter than that of MoKα may be processed, but those parts of the data processing requiring evaluation of atomic scattering factors will have dubious reliability because of the limitations of the Vand, Eiland, Pepinsky approximation equation for calculation of these quantities.

2.3 Data Reduction to the Form of Normalized Structure Factors

No limitations in addition to those above apply.

2.4 Data Reduction Extended to Include Ordering of $|E|^2 - 1$

The following limitations apply in addition to those above:

1. A maximum of 5000 unique reflections (including reflections for which $|E|^2 - 1 < 0$) can be accommodated in one pass. Of these 5000 reflections no more than 2400 can have $|E|^2 - 1 \geq 0$. Any number of passes may be made. Each pass orders 2400, or less, reflections independently of the reflections ordered in other passes. If there are more than 5000 reflections on the input tape, the program automatically orders the data in groups of 5000 (or less for the last group) until all of the data are ordered.

2. No more than 300 reflections can occur in any one of the eight groups segregated according to evenness or oddness of Miller indices for any one pass.

3. INPUT DATA AND FORMATS

3.1 Three Categories of Input Data

The input data are categorized into three main parts, each succeeding part being a subdivision of the preceding one, as follows:

I. General Information

General crystallographic and chemical information.

II. Crystal Setting Information

1. Information which defines an individual crystal setting.

2. Information which is pertinent, in general, only to all data collected from this setting.

III. Reciprocal Net Information

1. Information which defines an individual set of reflection data. This set of data consists of all of or part of the observable portion of a reciprocal lattice net obtained at the crystal setting specified in II.

2. Information which is pertinent in general, only to this particular set of data.

3. The reflection data.

The program user should understand clearly that the data in category I are specified only once for a given crystal. Category II data are specified for each crystal setting, and category III data are specified for each individual set or "layer" of data obtained at each setting.

In the exposition of the three categories given below, each type of card to be punched is treated in detail and is identified by number. A diagrammatic presentation of card composition with FORTRAN formats is included; the sequence of cards in the data deck is given last.

3.2 Category I - General Information

Card 1:

Card 1 is for input of Hollerith information, e.g., the name of the crystal and the name of the crystallographer. A maximum of 72 characters are allowed.

Card 2:

columns	1 - 11	12 - 22	23 - 33	34 - 44	45 - 55	56 - 66
data	A1	A2	A3	α1	α2	α3
format	F11.7	F11.7	F11.7	F11.7	F11.7	F11.7

Card 2 contains the "real-space" unit cell parameters in the order a, b, c, α, β, γ. The parameters a, b, and c are in units of angstroms; α, β, and γ are expressed in degrees and are always given, even when they are fixed by space group symmetry.

Card 3:

columns	1 - 12	13 - 24
data	R1	R2
format	E12.5	E12.5

Card 3 contains the x-ray beam collimator parameters R1 and R2 as defined by Phillips (1) for use in correcting intensity data for the expansion or compaction of spot size on upper layer equi-inclination Weissenberg photographs. For the standard Weissenberg goniometer these parameters have the values R1 = 28.648 and R2 = 78.000. Where this correction is not to be applied or is irrelevant, a blank card may be used.

Card 4:

columns	1 - 4	5 - 9
data	NS	S
format	I4	F5.4

Card 4 contains:

1. The number of different atomic species present in the crystal, NS.

2. The interval in $\sin^2\theta/\lambda^2$, S, to be used in calculating the log K curve for determination of the absolute base acale factor. The unit is angstrom^{-2}.

Card 5:

columns	1 - 8	9 - 16	17 - 24	25 - 32	33 - 40	41 - 44
data	A	a	B	b	C	NA
format	F8.4	F8.4	F8.4	F8.4	F8.4	F4.0

Card 5 is applicable to a single atomic species. There is a separate card for each species. The card contains:

1. The parameters A, a, B, b, and C as defined by Forsyth and Wells (8) for calculation of the atomic scattering factor. Values of these parameters are tabulated in the paper by Forsyth and Wells (see section 1.8).

2. The number of atoms of this atomic species in the unit cell, NA.

3.3 Category II – Crystal Setting Information

Card 6:

columns	1 - 3	4 - 6	7 - 9	10 - 12	13 - 15	16 - 26	27 - 37	38 - 48
data	U	V	W	ST	GT	RF	L	RS
format	F3.0	F3.0	F3.0	F3.0	F3.0	F11.8	F11.8	F11.8

Card 6 contains:

1. The zone axis indices U, V, W. As an example, consider a crystal mounted on its a axis. The zone axis indices for Weissenberg data would be 1, 0, 0. For the same crystal aligned on a precession goniometer so as to obtain the h0ℓ, h1ℓ, h2ℓ, etc. nets, the zone axis indices would be 0, 1, 0 (see section 2.1).

2. A test flag, ST, to answer the question: Is this the last setting to be read into the computer?

   Yes: ST = 1
   No: leave blank.

3. A test flag, GT, to answer the question: Is this Weissenberg or precession data?

   precession: GT = 1
   Weissenberg: leave blank.

4. The rejection factor, RF. In determing the average film factor (i.e., ratio of intensity estimates) between adjacent films in a pack, the ratios of all individual nonzero intensities appearing on both films are calculated and averaged. The product of this average and the "rejection factor" is the upper limit of acceptance of the ratios. The quotient of the average and the "rejection factor" is the lower limit of acceptance. Both intensity readings of a pair which yield a film factor falling outside the range of acceptance are rejected unless one of them also yields an acceptable film factor involving a third film. See section 1.3 for additional details.

5. Wavelength of x-radiation used, L, expressed in Angstrom units.

6. A value of $(\sin\theta)/\lambda$, RS, is specified at and above which the α_1 and α_2 spots are clearly resolved. Intensities of reflections with $(\sin\theta)/\lambda$ equal to or greater than this value are multiplied by 3/2. The unit is angstrom^{-1}.

Card 7:

columns	1 - 3	4 - 6	7 - 9	10 - 20	21 - 31
data	e	f	g	φ	$\bar{\mu}$
format	F3.0	F3.0	F3.0	F11.7	F11.7

Card 7 is included <u>if and only if</u> the data are obtained by the precession method. The card contains:

1. The net orientation indices e, f, g, which are the Miller indices of the lowest order reciprocal lattice point (even though its reflection may not appear on the film for any reason) lying on the upper half of the most nearly vertical central lattice line appearing in the zero layer reciprocal net (see section 2.1). This line is designated as the orientation axis. Its positive direction is upward. Horizontal, vertical, up, and down are relative to the goniometer base. (It is assumed that the Buerger type goniometer is used.)

2. The orientation axis angle φ, which is the angle between the positive orientation axis and the positive horizontal axis lying in the plane of the reciprocal net. The positive horizontal axis is directed away from the goniometer head. The angle is expressed in degrees.

3. The precession angle $\bar{\mu}$ expressed in degrees.

3.4 Category III - Reciprocal Net Information

Card 8:

columns	1 - 3	4 - 7	8 - 10	11 - 13	14 - 25
data	LN	NR	LT	PT	SF
format	F3.0	I4	F3.0	F3.0	E12.5

Card 8 contains:

1. The layer number, LN, i.e., the 0th, or 1st, or 2nd, etc., net above the zero level net.

2. Number of reflections included in the set, NR.

3. A test flag LT to answer the question: Is this the last set of data in this setting to be read into the computer?

Yes: LT = 1
No: leave blank.

4. A test flag PT to indicate, for Weissenberg data, whether the compacted or expanded spots were read in this set. For precession or integrated Weissenberg data, or other data for which the correction does not apply, the space is left blank.

compacted: PT = 1
ignore correction: leave blank
expanded: PT = - 1.

5. If two standard intensity scales have been used to estimate intensities, the data estimated with one of these scales are punched as negative numbers. This field contains the factor SF by which the negative data must be multiplied to bring them to the same scale as the data read by the other intensity scale. This factor is punched as a negative number. If only one standard scale has been used, this field is left blank.

Card 9:

columns	1 - 3	4 - 6	7 - 9	10 - 12	13 - 19	20 - 26	27 - 33	34 - 40	41 - 47	48 - 54	55 - 61
data	h	k	ℓ	ϵ	6	5	4	3	2	1	AB
format	I3	I3	I3	I3	F7.0	F7.0	F7.0	F7.0	F7.0	F7.0	F7.5

Card 9 contains individual reflection data. One card is punched for each reflection observed in the set. The number of cards in this set must equal NR as specified on Card 8 above. The card contains individual reflection data as follows:

1. The Miller indices h, k, and ℓ.

2. The integer factor ϵ which is the factor used to convert E^2 to $\mathcal{E}^2$. If the value of ϵ is 1, this field may be left blank.

3. Six fields containing the intensity readings from individual films either from separate exposures or from one or more film packs. There can be a maximum of six films. The fields are filled from right to left in order of decreasing exposure of the films. The sixth field from the left must contain the data from the most heavily exposed film. The fifth field from the left must contain the data from the secondmost heavily exposed film, etc. Where intensities are too strong or too weak to be estimated, the corresponding field is left blank, even when preceded or followed by nonzero fields. Where there are fewer than six films, the excess fields are left blank. If two intensity scales are used to estimate intensities, the data estimated from one of the scales are punched as negative numbers (see item 5 on card 8 above).

4. An absorption correction factor AB. This is the factor by which the individual intensity values must be multiplied to correct for absorption. If there are to be no corrections for absorption, this field may be left blank.

3.5 Sequence of Cards

The data deck is set up as follows:

General Information:	Card 1 Card 2 Card 3 Card 4 All cards 5
First Setting:	Card 6 Card 7 (if required)
First Set of Data:	Card 8 All cards 9
Second Set of Data:	Card 8 All cards 9
etc.	
Second Setting:	Card 6 Card 7 (if required)
First Set of Data:	Card 8 All cards 9
etc.	

4. OPERATING PROCEDURE

This section is divided into two parts. Section 4.1 is sufficient for those who intend to use the program but are not concerned with the operating procedure. Section 4.2 will add the details required for the operation of the program.

4.1 Instructions for the Crystallographer

The preceding portions of this exposition should be carefully studied to determine exactly what information is required, and how it is to be presented to the computer. It would be wise to do this before the work of estimating intensities is begun so that the reflection data is properly indexed and is recorded in a form convenient for key punching. The data sheet column headings, from left to right, should be h, k, ℓ, ϵ, 6, 5, 4, 3, 2, 1, AB (cf. formats for card 9 in section 3). The absorption correction factors, if any, should include decimal points. If no absorption correction factors are to be applied, their fields may be left blank. If intensity estimates expressed as integer numbers are right justified in their fields, decimal points need not be punched. Punched decimal points may appear anywhere within the fields.

Each independently observed set or "layer" of data must be handled individually throughout the processing. After each set of reflection data is punched, the cards are counted. This counting should be done mechanically to avoid human error.

The control cards (i.e., cards other than reflection cards) may be inserted in the deck after the individual sets of reflection cards have been stacked in the order in which they are to be loaded into the computer. The information on the control cards must be consistent with this ordering. In the usual case, the data deck will be loaded onto magnetic tape for input to the computer.

It is suggested that the data processing be approached in the following way:

Step 1. The data processing should be taken through (forced through if necessary) completion of the preliminary output. Any gross key punching or transcribing errors resulting in format inconsistencies, rejections of whole sets of data, or abnormal film factors should be detected at this stage. The preliminary output may be observed on the on-line printer. The reflection data are not required to be arranged in dictionary order of h, k, ℓ if the calculation is stopped at this point. Thus the first part of the calculation (DICNRY) may be omitted.

Step 2. After correction for the errors observed above, Step 1 is repeated, if necessary, in order to find all remaining detectable errors.

Step 3. A final check of the input tape (or deck) is made, by processing through the output of rejected reflections, prior to committing the data to complete processing. Prior to this calculation, it would be wise to spread the film factor acceptance limits to ensure that no additional rejections will occur. The newly computed film factors will be different from the old ones where corrections have been made. Consequently, some data, barely within the acceptable range in the prior calculation, may lie outside of that range in the final calculation.

Step 4. Finally, the processing is carried through to the farthest stage desired.

The BCD output tapes should be set aside for future use. If corrections to these tapes must be made, it will be necessary to have the data on them punched onto cards. The corrections are made on the cards, which then may be read back onto tape.

4.2 Instructions for the Machine Operator

The data reduction is divided into four separate calculations, labeled I, II, III, and IV, each involving independent read-in of its own program deck. These four calculations are discussed below and are diagrammed in Appendix A. Each successive calculation uses tapes prepared by the preceding calculation. To gain maximum efficiency the four calculations should be done in immediate succession.

BCD output for off-line printing is on tape 9. For XRDD, this output also may be observed on-line by depressing sense switch 6.

Tables 1 and 2 present summaries of the tape requirements and sense switch usage.

The complete FORTRAN source program listings are reproduced in Appendix B.

I. DICNRY (Dictionary Ordering of Data)

This program arranges the data within each set into dictionary order of h, k, and ℓ. It uses tapes 4 and 5.

Input is BCD either from tape 4 or from cards through the on-line card reader. If the on-line card reader input is used, depress sense switch 1.

The entire program output is on tape 5. This output is mostly binary but otherwise is identical with the input tape except that the data now are ordered within the sets. This tape serves as input to the next calculation.

Table 1
Summary of Tape Requirements

Program	Tape*	Input	Output	Inter-mediate	Binary	BCD
I. DICNRY	4	X				X
	5		X		X	X
II. XRDD	4		X		X	X
	5	X			X	X
	5		X			X
	6		X	X	X	
	7			X	X	
	7		X			X
	8		X	X	X	
	9†		X			X
III. SF NORM	4	X			X	X
	5		X			X
	6	X			X	
	7		X			X
	8	X			X	
	9†		X			X
IV. E ORDER	5	X				X
	9†		X			X

*As indicated in the Table, the individual tapes may serve several widely differing functions in the course of a calculation. Nevertheless, the same tapes can be used throughout. In practice, however, the user may wish to replace and save tapes 4 (input), 5 (input and output), and 7 (output) at certain stages of the processing (for example, see section 4.2, Calculation II).
†Tape 9 is used for BCD output to be printed off-line. It is never rewound by the program.

Table 2
Summary of Sense Switch Usage

Sense Switch	Usage
1	Down for card data input to DICNRY or XRDD.
2	Down for BCD tape data input to XRDD.
3	Down if data processing is to stop after preliminary output is completed.
4	Not used.
5	Not used.
6	Down for on-line printing of output from XRDD (this output is written on tape 9 regardless of the sense switch position).

The dictionary ordering calculation may be omitted entirely if the data cards are ordered prior to loading on tape. Ordinarily it will be omitted in the preliminary error detection runs.

II. XRDD (Data Reduction through the Output of Structure Factor Data)

This program uses tapes 4, 5, 6, 7, 8, and 9.

Tape 5 is used for input. Tape 5 may be either binary or BCD depending upon whether or not Calculation I has been done. If it is BCD, depress sense switch 2. If the input tape is to be saved, it must be replaced, or dialed out and another tape 5 dialed on, after the on-line printer reports that the preliminary averaging and Lp corrections have been completed. Usually, no interruption in the calculation is required for this replacement.

Alternatively, the data may be loaded through the on-line card reader. This mode of data loading is selected by depressing sense switch 1.

The data processing proceeds through the following stages:

1. Read-in of each set of data into the computer, calculation of average intensities, application of Lp corrections, and printout of film factors. This printout may be observed on-line by depressing sense switch 6.

2. Printout of rejected data. This printout may be observed on-line by depressing sense switch 6.

Notification of the completion of the processing to this stage will appear on the on-line printer. If sense switch 3 is down, calculation will stop at this point. To continue the calculation press the START button on the console.

3. Least-squares correlation of independently observed sets of data. Notification of completion of this calculation will appear on the on-line printer.

4. Final averaging and scaling. Notification of completion of these calculations will appear on the on-line printer. If sense switch 6 is down at this time, the on-line printer will print notification of this fact and the calculation will stop. To continue, with sense switch 6 up or down, push START.

5. Structure factor output. This may be observed on-line by depressing sense switch 6. Notification of completion of the output will appear on the on-line printer.

Tapes 5 and 7 are BCD output tapes ready for input to the Busing least-squares refinement program (see section 1.10). Tape 5 contains the averaged data and tape 7 contains the unaveraged data. If the data processing is to be extended to include Calculation III (calculation and output of normalized structure factors), these tapes must be replaced and saved before Calculation III is begun.

Tapes 4, 6, and 8 are used as input to Calculation III.

III. SF NORM (Normalization of Structure Factors)

This program uses tapes 4, 5, 6, 7, 8, and 9. Tapes 4, 6, and 8 are the same tapes 4, 6, and 8 involved in Calculation II above.

Tapes 5 and 7 are BCD output tapes ready for input to the Fourier program of Sly and Shoemaker. Tape 5 contains the averaged data, and tape 7 contains the unaveraged data.

Notification that both the calculation and output have been completed will appear on the on-line printer.

Either tape 5 or 7 may be used as input to Calculation IV, but tape 5 usually will be used.

IV. E ORDER (Ordering of $|E|^2 - 1$ Data)

This program uses tape 5 for input. This tape is either tape 5 or tape 7 from the output of Calculation III. No other tapes are used. The contents of the input tape are not altered. Output is on tape 9.

The program processes 5000 or less reflection data per pass. If there are more than 5000 data on the input tape, the program processes the data in groups of 5000 until all are done (see section 2.4).

Notification of completion of the calculation will appear on the on-line printer.

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APPENDIX A

FLOW DIAGRAMS OF THE FOUR SUCCESSIVE CALCULATIONS

The four diagrams which follow indicate the main stream of flow of the data processing for the four separate calculations. The long-dash boxes enclose the portions of the calculations under control of the FORTRAN executive programs. FORTRAN subroutines are enclosed in short-dash boxes. The subroutine names are found in the upper left corners of the boxes.

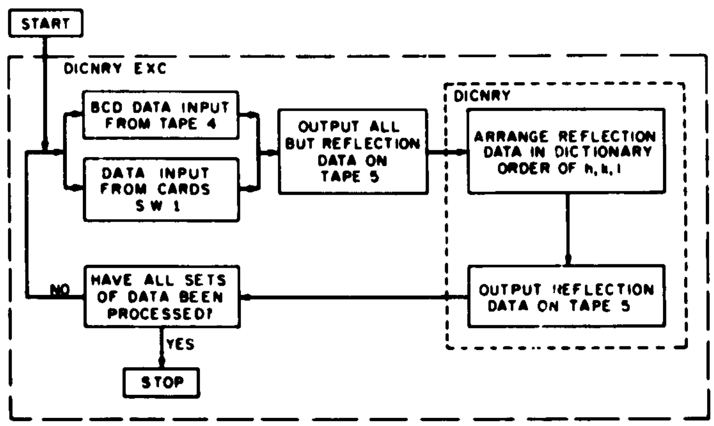

Fig. A1 - Calculation I

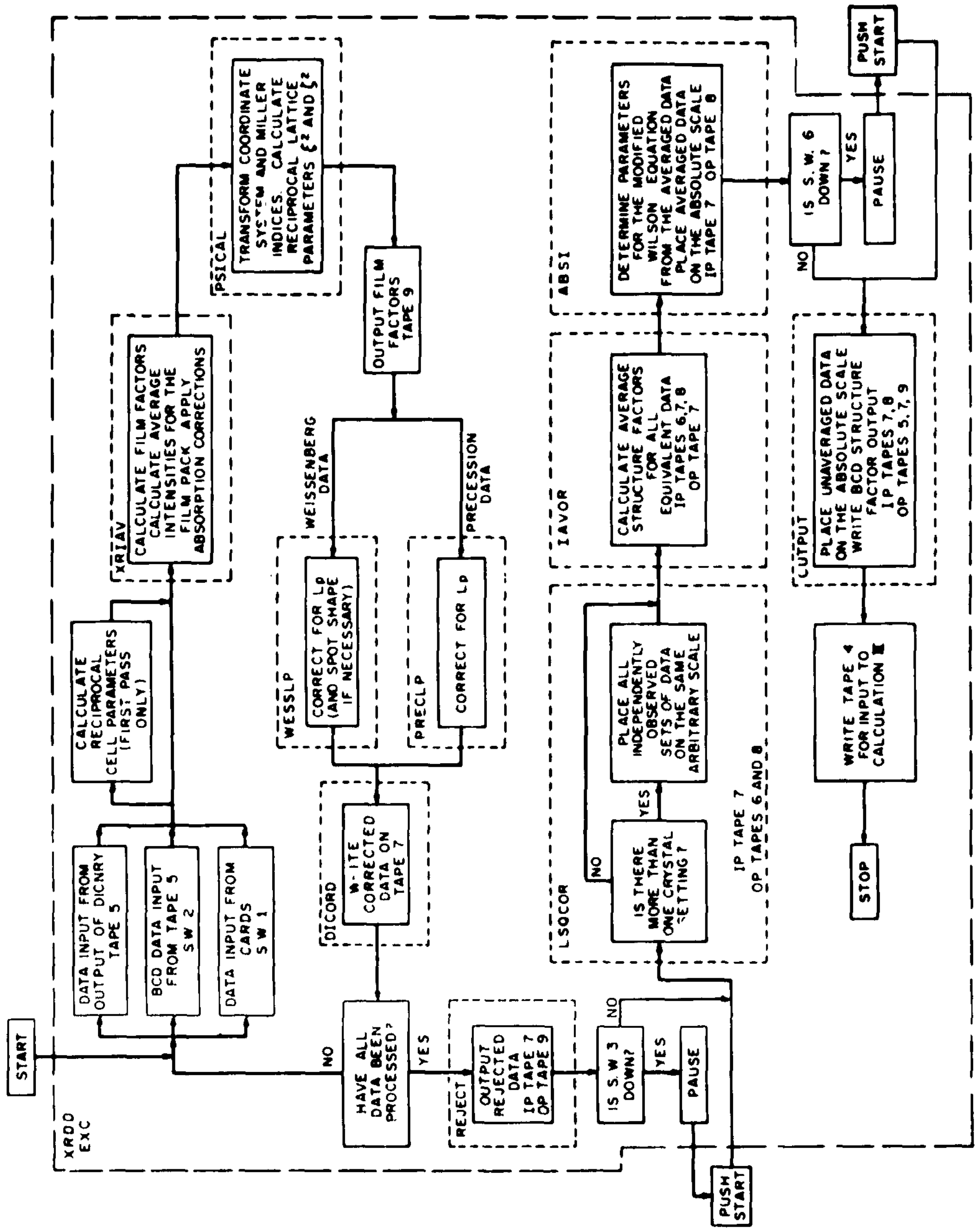

Fig. A2 - Calculation II

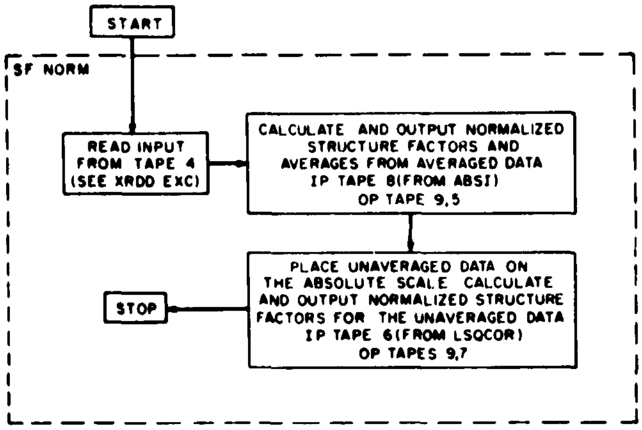

Fig. A3 - Calculation III

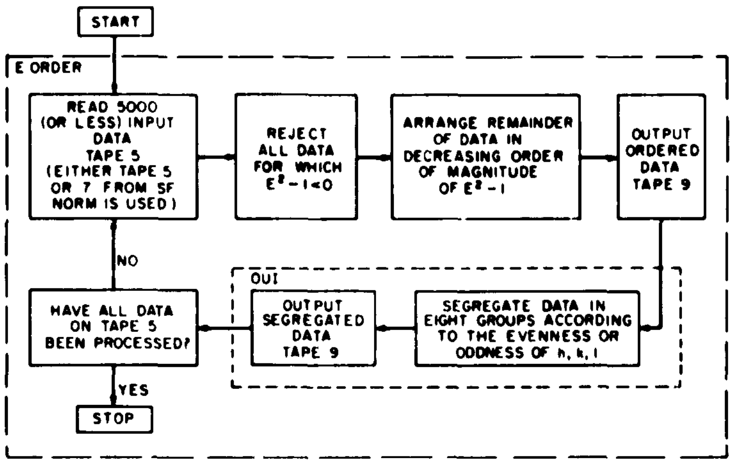

Fig. A4 - Calculation IV

APPENDIX B

COMPLETE FORTRAN SOURCE PROGRAM LISTINGS

The complete FORTRAN source program listings are reproduced in this appendix.

FUNCTION INTG is called by both XRDD EXC and SF NORM.

```
C     DICNRY FXC
      DIMENSION Q(6,1000),L1(1000),L2(1000),L3(1000),LPS(1000),ABSC
     1(1000),AS(20),AS1(20),BS(20),BS1(20),CS(20),AN(20)
      COMMON L1,L2,L3,LPS,Q,ABSC
      REWIND 4
      REWIND 5
      IF(SENSE SWITCH 1)100,200
  100 READ 5
      READ 10,AR,BR,CR,ALR,BER,GAR
      READ 20,R1,R2
      READ 30,NASP,S2I
      READ 40,(AS(I),AS1(I),BS(I),BS1(I),CS(I),AN(I),I=1,NASP)
      GO TO 300
  200 READ INPUT TAPE 4,5
      READ INPUT TAPE 4,10,AR,BR,CR,ALR,BER,GAR
      READ INPUT TAPE 4,20,R1,R2
      READ INPUT TAPE 4,30,NASP,S2I
      READ INPUT TAPE 4,40,(AS(I),AS1(I),BS(I),BS1(I),CS(I),AN(I),I=1,
     1NASP)
  300 WRITE OUTPUT TAPE 5,5
      WRITE OUTPUT TAPE 5,10,AR,BR,CR,ALR,BER,GAR
      WRITE        TAPE 5   ,R1,R2
      WRITE        TAPE 5   ,NASP,S2I
      WRITE        TAPE 5   ,(AS(I),AS1(I),BS(I),BS1(I),CS(I),AN(I),I=1,
     1NASP)
  105 IF(SENSE SWITCH 1)110,210
  110 READ 50,U1,U2,U3,CE,PE,REJ,YAM,SINH
      IF(PE)310,310,120
  120 READ 60,E1,E2,E3,PHI,UM
      GO TO 310
  210 READ INPUT TAPE 4,50,U1,U2,U3,CE,PE,REJ,YAM,SINH
      IF(PE)310,310,220
  220 READ INPUT TAPE 4,60,E1,E2,E3,PHI,UM
  310 WRITE        TAPE 5   ,U1,U2,U3,CE,PE,REJ,YAM,SINH
      IF(PE)330,330,320
  320 WRITE        TAPE 5   ,E1,E2,E3,PHI,UM
  330 IF(SENSE SWITCH 1)130,230
  130 READ 70,SL,NR,TL,BSE,SFI
      READ 80,(L1(I),L2(I),L3(I),LPS(I),(Q(J,I),J=1,6),ABSC(I),I=1,NR)
      GO TO 340
  230 READ INPUT TAPE 4,70,SL,NR,TL,BSE,SFI
      READ INPUT TAPE 4,80,(L1(I),L2(I),L3(I),LPS(I),(Q(J,I),J=1,6),
     1ABSC(I),I=1,NR)
  340 WRITE        TAPE 5   ,SL,NR,TL,BSE,SFI
  350 CALL DICNRY(NR)
  360 IF(TL)330,330,370
  370 IF(CE)105,105,380
  380 REWIND 4
      REWIND 5
      PRINT 90
      PAUSE
    5 FORMAT(72H
     1         )
   10 FORMAT(6F11.7)
```

```
20 FORMAT(2E12.5)
30 FORMAT(I4,F5.4)
40 FORMAT(5F8.4,F4.0)
50 FORMAT(5F3.0,3F11.8)
60 FORMAT(3F3.0,2F11.7)
70 FORMAT(F3.0,I4,2F3.0,F12.5)
80 FORMAT(4I3,6F7.0,F7.5)
90 FORMAT(62H JOB FINISHED.. INPUT FOR DATA REDUCTION PROGRAM IS ON
  1APE 5. ////////// )
   END(1,1,0,0,1)
```

```
      SUBROUTINE DICNRY(NR)
      DIMENSION Q(6,1000),L1(1000),L2(1000),L3(1000),LPS(1000),ABSC
     1(1000),M2(1000),M3(1000),K1(1000),N1(1000),N2(1000),N3(1000),NI
     2(1000),Q1(6,1000),ABSC1(1000),J3(100),K2(100)
      COMMON L1,L2,L3,LPS,Q,ABSC,N1,N2,N3,NPS1,Q1,ABSC1
      FREQUENCY 100(300),110(2,1,5),140(300),150(2,1,5),180(300),
     1190(5,1,5),211(0,1,5),220(100),230(5,1,2),260(100),270(5,1,2),
     2300(100),310(5,1,5),331(0,1,5),340(25),350(5,1,2),380(25),390
     3(5,1,2),430(5,1,5),470(25),460(1,1,5),470(1,1,5),480(1,1,5)
      L=0
      MS1=L1(1)
  100 DO 130 I=1,NR
  110 IF(L1(I)-MS1)120,130,130
  120 MS1=L1(I)
  130 CONTINUE
      IG1=L1(1)
  140 DO 170 I=1,NR
  150 IF(IG1-L1(I))160,170,170
  160 IG1=L1(I)
  170 CONTINUE
  175 MK=0
  180 DO 210 I=1,NR
  190 IF(MS1-L1(I))210,200,210
  200 MK=MK+1
      M2(MK)=L2(I)
      M3(MK)=L3(I)
      K1(MK)=I
  210 CONTINUE
  211 IF(MK)490,490,215
  215 MS2=M2(1)
  220 DO 250 I=1,MK
  230 IF(MS2-M2(I))250,250,240
  240 MS2=M2(I)
  250 CONTINUE
      IG2=M2(1)
  260 DO 290 I=1,MK
  270 IF(M2(I)-IG2)290,290,280
  280 IG2=M2(I)
  290 CONTINUE
  295 ML=0
  300 DO 330 I=1,MK
  310 IF(MS2-M2(I))330,320,330
  320 ML=ML+1
      J3(ML)=M3(I)
      K2(ML)=K1(I)
  330 CONTINUE
  331 IF(ML)470,470,335
  335 MS3=J3(1)
  340 DO 370 I=1,ML
  350 IF(MS3-J3(I))370,370,360
  360 MS3=J3(I)
  370 CONTINUE
      IG3=J3(1)
  380 DO 410 I=1,ML
```

```
390 IF(J3(I)-IG3)410,410,400
400 IG3=J3(I)
410 CONTINUE
420 DO 450 I=1,ML
430 IF(MS3-J3(I))450,440,450
440 M=K2(I)
    L=L+1
    N1(L)=MS1
    N2(L)=MS2
    N3(L)=MS3
    NPS1(L)=LPS(M)
    DO 445 K=1,6
445 Q1(K,L)=Q(K,M)
    ABSC1(L)=ABSC(M)
450 CONTINUE
    MS3=MS3+1
460 IF(IG3-MS3)470,420,420
470 MS2=MS2+1
480 IF(IG2-MS2)490,295,295
490 MS1=MS1+1
500 IF(IG1-MS1)510,175,175
510 WRITE        TAPE 5   ,(N1(I),N2(I),N3(I),NPS1(I),(Q1(K,I),K=1,6),
   1ABSC1(I),I=1,NR)
 80 FORMAT(4I3   ,6F7.1,F7.4)
    RETURN
    END(2,2,2,2,2)
```

```
      XRDD EXC
      DIMENSION Q(6,1000),H1(1000),H2(1000),H3(1000),EPS(1000),AVEQ(1000
     1),REJQ(1000),RENO(1000),ABSC(1000),AVSE(5),NPS(1000),AS(20),BS(20)
     2,CS(20),AS1(20),BS1(20),AN(20),SMYAM(10),N1(1000),N2(1000),
     3 N3(1000)
      COMMON H1,H2,H3,EPS,AVEQ,REJQ,RENO,ABSC,Q,N1,N2,N3,NPS
      FREQUENCY 105(0,3,1),125(0,3,1),155(0,3,1),160(0,2,1),172(2)
    5 FORMAT(72H
     1             )
   10 FORMAT(6F11.7)
   20 FORMAT(2E12.5)
   30 FORMAT(I4,F5.4)
   40 FORMAT(5F8.4,F4.0)
   50 FORMAT(5F3.0,3F11.8)
   60 FORMAT(3F3.0,2F11.7)
   70 FORMAT(F3.0,I4,2F3.0,E12.5)
   80 FORMAT(4F3.0,6F7.0,F7.5)
  500 FORMAT(1H ,41H LEAST SQUARES LAYER CORRELATION FINISHED/////)
  510 FORMAT(1H ,25H FINAL AVERAGING FINISHED/////)
  520 FORMAT(1H ,88H DATA REDUCTION FINISHED. RELEASE SENSE SWITCH 6 AND
     1CONTINUE FOR LOADING OF OUTPUT TAPES/////)
  530 FORMAT(1H1)
   90 FORMAT(1H ,49HPRELIMINARY AVERAGING AND LP CORRECTIONS FINISHED///
     1//)
  540 FORMAT(113H REPLACE AND SAVE TAPES 5 AND 7.               READ I
     1N JOB    SF  NORM    FOR CALC. AND OUTPUT OF E AND E**2-1.////////
     2///)
  550 FORMAT(1H0,3I4,8H   LAYERI3,I8)
  560 FORMAT(1H0)
  570 FORMAT(1H0,102H                                 5              4
     1                3                 2                 1)
  580 FORMAT(1H0,18H   FILM FACTORS   5E18.7)
  590 FORMAT(68H DATA REDUCTION FINISHED.  LOADING OF OUTPUT TAPES WILL
     1NOW PROCEED./////)
      REWIND 4
      IF(SENSE SWITCH 1)1000,900
  900 IF(SENSE SWITCH 2)902,901
  902 NNN=2
      GO TO 1001
 1000 READ 5
      READ 10,AR,BR,CR,ALR,BER,GAR
      NNN=3
      GO TO 1002
  901 NNN=1
 1001 REWIND 5
      READ INPUT TAPE 5,5
      READ INPUT TAPE 5,10,AR,BR,CR,ALR,BER,GAR
 1002 ALR=ALR*3.14159/180.0
      BER=BER*3.14159/180.0
      GAR=GAR*3.14159/180.0
      COSAR=COSF(ALR)
      COSBR=COSF(BER)
      COSGR=COSF(GAR)
      VR=AR*BR*CR*SQRTF(1.0-COSAR*COSAR-COSBR*COSBR-COSGR*COSGR+2.*COSAR
```

```
    1*COSBR*COSGR)
     SINAR=SINF(ALR)
     SINBR=SINF(BER)
     SINGR=SINF(GAR)
     AA=BR*CR*SINAR/VR
     BB=AR*CR*SINBR/VR
     CC=AR*BR*SINGR/VR
     COSAL=(COSBR*COSGR-COSAR)/(SINBR*SINGR)
     COSBE=(COSAR*COSGR-COSBR)/(SINAR*SINGR)
     COSGA=(COSAR*COSBR-COSGR)/(SINAR*SINBR)
     GO TO (903,1004,1003),NNN
1003 READ 20,R1,R2
     READ 30,NASP,S2I
     READ 40,(AS(I),AS1(I),BS(I),BS1(I),CS(I),AN(I),I=1,NASP)
     GO TO 1005
1004 READ INPUT TAPE 5,20,R1,R2
     READ INPUT TAPE 5,30,NASP,S2I
     READ INPUT TAPE 5,40,(AS(I),AS1(I),BS(I),BS1(I),CS(I),AN(I),
    1 I=1,NASP)
     GO TO 1005
 903 READ       TAPE 5    ,R1,R2
     READ       TAPE 5    ,NASP,S2I
     READ       TAPE 5    ,(AS(I),AS1(I),BS(I),BS1(I),CS(I),AN(I),
    1 I=1,NASP)
1005 ZETA=0.0
     ONE23=0.0
     COSGA1=0.0
     A=0.0
     B=0.0
     C=0.0
     A1=0.0
     A2=0.0
     A3=0.0
     NOZ=0
     EX=0.0
     SF=0.0
     NI=0
     NSET=0
     NS=0
     BT1=0.0
     BT2=0.0
     NRT=0
     DO 95 J=1,5
  95 AVSF(J)=0.0
     PRINT 530
     REWIND 7
 100 GO TO(904,1007,1006),NNN
1006 READ 50,U1,U2,U3,CE,PE,REJ,YAM,SINH
     GO TO 1008
1007 READ INPUT TAPE 5,50,U1,U2,U3,CE,PE,REJ,YAM,SINH
     GO TO 1008
 904 READ       TAPE 5    ,U1,U2,U3,CE,PE,REJ,YAM,SINH
1008 NSET=NSET+1
     SMYAM(NSET)=YAM
```

```
      SINH=SINH**2
 105  IF(PE)120,120,110
 110  GO TO(905,1010,1009),NNN
1009  READ 60,E1,E2,E3,PHI,UM
      GO TO  1011
1010  READ INPUT TAPE 5,60,E1,E2,E3,PHI,UM
      GO TO 1011
 905  READ        TAPE 5   ,E1,E2,E3,PHI,UM
1011  PHI=PHI*3.14159/180.0
      UM=UM*3.14159/180.0
 120  GO TO(906,1013,1012),NNN
1012  READ 70,SL,NR,TL,BSE,SFI
      READ 80,(H1(I),H2(I),H3(I),EPS(I),(Q(J,I),J=1,6),ABSC(I),I=1,NR)
      GO TO 1014
1013  READ INPUT TAPE 5,70,SL,NR,TL,BSE,SFI
      READ INPUT TAPE 5,80,(H1(I),H2(I),H3(I),EPS(I),(Q(J,I),J=1,6),
     1 ABSC(I),I=1,NR)
      GO TO 1014
 906  READ        TAPE 5   ,SL,NR,TL,BSE,SFI
      READ        TAPE 5   ,(N1(I),N2(I),N3(I),NPS(I),(Q(J,I),J=1,6),
     1 ABSC(I),I=1,NR)
      DO 907 I=1,NR
      H1(I)=N1(I)
      H2(I)=N2(I)
      H3(I)=N3(I)
      IF( ABSC(I)) 1907,1906,1907
1906  ABSC(I) =1.0
1907  IF(NPS(I)) 907,1908,907
1908  NPS(I) =1
 907  EPS(I)=NPS(I)
1014  MSL=INTG(SL)
      MU1=INTG(U1)
      MU2=INTG(U2)
      MU3=INTG(U3)
      NRT=NRT+NR
      WRITE OUTPUT TAPE 9,560
      WRITE OUTPUT TAPE 9,550,MU1,MU2,MU3,MSL,NR
      IF(SENSESWITCH 6)1015,1016
1015  PRINT 560
       PRINT 550,MU1,MU2,MU3,MSL,NR
1016  NS=NS+1
      CALL XRIAV(SFI,NR,REJ,AVSE)
      CALL PSICAL(AA,BB,CC,COSAL,COSBE,COSGA,NR,YAM,U1,U2,U3,SL,ZETA,
     1ONE23,COSGA1,A,B,C,A1,A2,A3)
      WRITE OUTPUT TAPE 9,570
      WRITE OUTPUT TAPE 9, 580,(AVSE(J),J=1,5)
      IF(SENSESWITCH 6) 1017,125
1017  PRINT 570
      PRINT 580,(AVSE(J),J=1,5)
 125  IF(PE)140,140,130
 130  CALL PRECLP(E1,E2,E3,COSAL,COSBE,COSGA,U1,U2,U3,PHI,COSGA1,NR,UM,
     1 YAM,ONE23,ZETA,A,B,C,A1,A2,A3,SINH)
      GO TO 150
 140  CALL WESSLP(YAM,NR,R1,R2,SINH,ZETA,BSE)
```

```
 150 CALL DICORD(U1,U2,U3,CE,PE,SL,NR,TL)
 155 IF(TL)120,120,160
 160 IF(CE)100,100,170
 170 CALL REJECT(NS)
     PRINT 90
     IF(SENSE SWITCH 3)1701,1702
1701 PAUSE
1702 REWIND 5
     CALL LSQCOR(NS)
     PRINT 500
     CALL IAVOR(NS,NOZ)
     PRINT 510
     SYAM=SMYAM(1)
 172 DO 180 I=1,NSET
     IF(SYAM-SMYAM(I))180,180,175
 175 SYAM=SMYAM(I)
 180 CONTINUE
     CALL ABSI(SYAM,AS,BS,CS,AS1,BS1,NASP,AN,S2I,NOZ,EX,SF,NI,BT1,BT2)
     IF(SENSE SWITCH 6)190,200
 190 PRINT 520
     PAUSE
     GO TO 210
 200 PRINT 590
 210 WRITE OUTPUT TAPE 9,530
     WRITE OUTPUT TAPE 9,5
     IF(SENSESWITCH 6)211,212
 211 PRINT 530
     PRINT 5
 212 CALL OUTPUT(NOZ,NS,NI,BT1,BT2,SF,EX,NOIB)
     WRITE OUTPUT TAPE 4,5
     WRITE TAPE 4,NASP
     WRITE TAPE 4,(AS(I),AS1(I),BS(I),BS1(I),CS(I),AN(I),I=1,NASP)
     WRITE TAPE 4,NOZ,NS,NI,BT1,BT2,SF,EX,NOIB,NRT
     REWIND 4
     PRINT 540
     PAUSE
     END(0,1,0,0,1)
```

```
      SUBROUTINE XRIAV (SFI,NR,REJ,AVSE)
      DIMENSION Q(6,1000),SE(5,1000),AVSE(5),REJQ(1000),RENO(1000),
     1H1(1000),      AVEQ(1000), ABSC(1000),H2(1000),H3(1000),
     1 EPS(1000)
      COMMON H1,H2,H3,EPS,AVEQ,REJQ,RENO
      COMMON ABSC,Q,SE
      FREQUENCY 130(300),140(1,4,12),80(1,4,12),200(300),205(0,1,3),
     1          20(0,1,3),222(300),223(1,0,20),225(1,0,20),245(300),
     1        246(1, 6, 14),285(300),286(1,6,14),315(1,6,14),
     1        340(0,1,3) ,224(0,1,1),325 (0,1,1)
  130 DO 195 I=1,NR
      DO 190 J =1,5
  140 IF(Q(J,I)) 170,150,180
  150  SE(J,I)  = 0.0
  160  GO TO 190
  170  Q(J,I) =   SFI *  Q(J,I)
  180  SE(J,I) =  Q(J+1,I) / Q(J,I)
   80 IF(SE(J,I)) 181 , 190,190
  181 SE(J,I) =  SFI  * SE(J,I)
  190 CONTINUE
   90 IF(Q(6,I))191,195,195
  191 Q(6,I)=Q(6,I)*SFI
  195 CONTINUE
      DO 270  J=1,5
      LUMP=0
      SIGMA1    = 0.0
      SIGMA2    = 0.0
  200 DO 220 I = 1,NR
  205 IF(SE(J,I)) 220,220,210
  210 SIGMA1   =SE(J,I) +SIGMA1
      SIGMA2   =1.0 + SIGMA2
  220 CONTINUE
   20 IF(SIGMA2)   21,21,221
   21 AVSE(J)=0.0
      GO TO 270
  221 AVSE(J) = SIGMA1   / SIGMA2
      REJH    =  AVSE(J) * REJ
      REJL    =  AVSE(J) / REJ
  222 DO 240  I=1,NR
  223 IF(REJH    - SE(J,I)) 230,230,224
  224 IF(SE(J,I))240,240,225
  225 IF(SE(J,I) - REJL    ) 230,230,240
  230 SE(J,I) = -1.0
      LUMP=1
  240 CONTINUE
      IF(LUMP)270,270,241
  241 SIGMA1=0.0
      SIGMA2=0.0
      LUMP=0
  245 DO 260  I = 1,NR
  246 IF(SE(J,I)) 260,260,250
  250 SIGMA1    = SE(J,I) + SIGMA1
      SIGMA2    = 1.0 + SIGMA2
  260 CONTINUE
```

```
    GO TO 221
270 CONTINUE
275 DO 280 J=1,4
    N = J + 1
276 DO 280  L= N,5
280 AVSE(J) = AVSE(J) *  AVSE(L)
285 DO 370  I = 1,NR
    SUMQ    = 0.0
    REJQ(I) = 0.0
    RENO(I) = 0.0
    DO 310  J = 1,5
286 IF(SE(J,I)) 287,290,300
287 IF(J - 1) 289,289,288
288 IF(SE(J-1,I))289,289,300
289 REJQ(I)  = 1.0
    GO TO 310
290 IF(Q(J,I))310,310,291
291 IF(J-1)300,300,292
292 IF(SE(J-1,I))310,300,300
300 SUMQ    =  Q(J,I) * AVSE(J) + SUMQ
    RENO(I) =  RENO(I) + 1.0
310 CONTINUE
315 IF(SE(5,I)) 320,325,330
320 REJQ(I) = 1.0
    GO TO 340
325 IF(Q(6,I))340,340,330
330 SUMQ    =  SUMQ    + Q(6,I)
    RENO(I) =  RENO(I) + 1.0
340 IF(RENO(I))350,350,360
350 AVEQ(I) = 0.0
    GO TO 370
360 AVEQ(I) =  SUMQ   *ABSC(I) / RENO(I)
370 CONTINUE
    FREQUENCY 287(0,1,6),288(5,1,5),290(0,10,1),291(0,1,6),
   1           292(1,10,3),90(1,4,12)
    RETURN
    END(1,1,0,0,0)
```

```
      SUBROUTINE PSICAL (AA,BB,CC,COSAL,COSBE,COSGA,NR,YAM,U1,U2,U3,SL,
     1 ZETA,ONE23,COSGA1,A,B,C,A1,A2,A3)
      DIMENSION X1(1000),X2(1000),X3(1000),H1(1000),H2(1000),H3(1000),
     1SI(1000), PSI(1000),AVEQ(1000),REJQ(1000),RENO(1000),PL(1000)
     1 ,EPS(1000)
      COMMON H1,H2,H3,EPS,AVEQ,REJQ,RENO
      COMMON PSI,PL,SI
      COMMON X1,X2,X3
      FREQUENCY 400(1,30,10),410(1,30,10),420(1,30,10),435(300),
     1        455(300),475(300),495(300)
      A = AA * YAM
      B = BB * YAM
      C = CC * YAM
      A11= SQRTF((U1*B)**2 +(U2*A)**2 + 2.0*(U1*B)*(U2*A)*COSGA)
      A12= SQRTF((U3*B)**2 +(U2*C)**2 + 2.0*(U3*B)*(U2*C)*COSAL)
      A21= SQRTF((U3*A)**2 +(U1*C)**2 + 2.0*(U3*A)*(U1*C)*COSBE)
      A3 = SQRTF((U1*A)**2 +(U2*B)**2 +(U3*C)**2
     1 + 2.0*((U1*A)*(U2*B)*COSGA    +(U1*A)*(U3*C)*COSBE
     2 +(U2*B)*(U3*C)*COSAL))
      BDOTC1 = U1*U3*(A*A-C*C)+U2*U3*A*B*COSGA
     1   +(U3*U3 - U1*U1)*A*C* COSBE  - U1*U2*B*C* COSAL
      ADOTC1 = U1*U2*(A*A  - B*B ) + (U2*U2 - U1*U1)*A*B*COSGA
     1    + U2*U3*A*C*COSBE - U1*U3*B*C*COSAL
      ADOTC2 =  U2*U3*(C*C  - B*B ) + U1*U2*A*C*COSBE - U1*U3*A*B*COSGA
     1  +(U2*U2 - U3*U3)*B*C*COSAL
      UV   = U1*U2
      U2W2 = U1*U1 + U3*U3
      VW   = U2*U3
      UW   = U1*U3
      U2V2 = U1*U1 + U2*U2
      V2W2 = U2*U2 + U3*U3
      UVW  =1.0/(U1*U1 + U2*U2 + U3*U3)
  400 IF(U1)430,410,430
  410 IF(U2)420,450,420
  420 IF(U3)430,470,430
  430 UUVW=UVW/U1
      ADOTB1 =    VW *A*A  -   UV *A*C*COSBE -   UW *A*B*COSGA
     1    +U1*U1*B*C*COSAL
      ONE23 = -1.0
      COSAL1 =  BDOTC1 / (A21* A3 )
      COSBE1 =  ADOTC1 / (A11* A3 )
      COSGA1 = ADOTB1 / (A11* A21)
      A1 = A11
      A2 = A21
  435 DO 440  I = 1,NR
      X1(I)=(H1(I)*UV - H2(I)* U2W2 + H3(I)*VW)* UUVW
      X2(I)=(H1(I)*UW + H2(I)*VW - H3(I)*U2V2)* UUVW
  440 X3(I)=(H1(I)*U1 + H2(I)*U2 + H3(I)*U3)* UVW
      GO TO 490
  450 ADOTB2 =  -UV*C*C  +VW*A*C*COSBE - U3*U3*A*B*COSGA +UW*B*C*COSAL
      ONE23 = 0.0
      COSAL1 =  BDOTC1 /(A21*A3 )
      COSBE1 =  ADOTC2 /(A12*A3 )
      COSGA1 =  ADOTB2 /(A12*A21)
```

```
    WUVW=UVW/U3
    A1 = A12
    A2 = A21
455 DO460  I= 1,NR
    X1(I)= (H1(I)*UV - H2(I)*U2W2 + H3(I)*VW)* WUVW
    X2(I)= (H1(I)*V2W2 - H2(I)*UV - H3(I)*UW)* WUVW
460 X3(I)= (H1(I)* U1 + H2(I)*U2 + H3(I)*U3)* UVW
    GO TO 490
470 ADOTB3 =  -UW*B*B  + VW*A*B*COSGA - U2*U2*A*C*COSBE +UV*B*C*COSAL
    ONE23 = 1.0
    COSAL1 =  - ADOTC2/(A12* A3)
    COSBE1 =    ADOTC1/(A11* A3)
    COSGA1 =    ADOTB3/(A11* A12)
    VUVW=UVW/U2
    A1 = A11
    A2 = A12
475 DO480   I = 1,NR
    X1(I) = (H1(I)*V2W2  - H2(I)*UV - H3(I)*UW)* VUVW
    X2(I) = (H1(I)*UW + H2(I)*VW - H3(I)*U2V2)* VUVW
480 X3(I) = (H1(I)*U1 + H2(I)*U2 + H3(I)*U3)* UVW
490 SIN2A1 = 1.0 - COSAL1*COSAL1
    SIN2B1 = 1.0 - COSBE1*COSBE1
    SIN2G1 = 1.0 - COSGA1*COSGA1
    ZETA  =(SL*A3)**2 *  SIN2B1*(1.0 -( COSAL1 - COSBE1*COSGA1)**2
   1  /(SIN2G1*SIN2B1))
    DEL = SL*A3*(SIN2G1*COSBE1 - COSGA1*(COSAL1 - COSGA1*COSBE1))/
   1      SIN2G1
    EPSI = SL*A3*(COSAL1-COSGA1*COSBE1)/SIN2G1
495 DO 500  I=1,NR
    IF(X3(I))496,500,500
496 X1(I)=-X1(I)
    X2(I)=-X2(I)
    X3(I)=-X3(I)
500 PSI(I) =(X1(I)*A1 + DEL)**2 + (X2(I)*A2 + EPSI)**2
   1   + 2.0*(X1(I)*A1+DEL)*(X2(I)*A2 + EPSI)*COSGA1
    RETURN
    END(1,1,0,0,0)
```

```
      SUBROUTINE PRECLP(E1,E2,E3,      COSAL,COSBE,COSGA,U1,U2,U3,
     1 PHI,COSGA1,NR,UM,YAM,ONE23,ZETA,A,B,C,A1,A2,A3,SINH)
      DIMENSION  COST(1000),SINT(1000),X1(1000),X2(1000),X3(1000),
     1     PSI(1000),PL(1000),SI(1000),AVEQ(1000),H1(1000),H2(1000),
     1 H3(1000),EPS(1000),REJQ(1000),RENO(1000)
      FREQUENCY 5(2,1,1),50(1,0,1),65(2,1,1),80(1,0,1),90(1,0,1),
     1          145(300),165(2,1,1),180(1,0,1),190(1,0,1),255(300),
     1          275(300)
      COMMON H1,H2,H3,EPS,AVEQ,REJQ,RENO
      COMMON PSI,PL,SI
      COMMON X1,X2,X3
      COMMON COST,SINT
      VER =SQRTF((E1*A)*(E1*A) + (E2*B)*(E2*B) + (E3*C)*(E3*C)
     1   + 2.0*((E1*A)*(E2*B)*COSGA +(E1*A)*(E3*C)*COSBE +
     1        (E2*B)*(E3*C)*COSAL))
      VDOTA1=E1*U2*A*A - E2*U1*B*B + (E2*U2 - E1*U1)*A*B*COSGA
     1            + E3*U2*A*C*COSBE - E3*U1*B*C*COSAL
      VDOTB1= E1*U3*A*A - E3*U1*C*C + E2*U3*A*B*COSGA
     1          +(E3*U3 - E1*U1)*A*C*COSBE - E2*U1*B*C*COSAL
      VDOTA2=  - E2*U3*B*B + E3*U2*C*C - E1*U3*A*B*COSGA
     1          + (E2*U2 - E3*U3)*B*C*COSAL + E1*U2*A*C*COSBE
    5 IF(ONE23) 10,20,30
   10 VDOTA = VDOTA1
      VDOTB = VDOTB1
      GO TO 40
   20 VDOTA =  VDOTA2
      VDOTB =  VDOTB1
      GO TO 40
   30 VDOTA  = VDOTA1
      VDOTB  = - VDOTA2
   40 IF(1.0-ABSF(COSGA1))42,42,45
   42 SINGA1=0.0
      GO TO 46
   45 SINGA1 = SQRTF (1.0 - COSGA1* COSGA1)
   46 COSVA =VDOTA/(A1* VER)
      COSVB =VDOTB/(A2 * VER)
      CVA1 =  E3*(U1*U1 +U2*U2) - U3*(U1*E1 + U2*E2)
      CVB1 =  U2*(U3*E3 + U1*E1) - E2*(U1*U1 + U3*U3)
      CVA2 =  U1*(UI*E2 + U3*E3) - E1*(U2*U2 + U3*U3)
      COSPH = COSF(PHI)
      SINPH = SINF(PHI)
   50 IF(ABSF(COSVA) - ABSF(COSVB)) 60,160,160
   60 IF(1.0-ABSF(COSVB))62,62,63
   62 SINVB=0.0
      GO TO 66
   63 SINVB = SQRTF( 1.0 - COSVB * COSVB)
   66 CAPHVB =  COSPH * COSVB   -   SINPH * SINVB
      SAPHVB =  SINPH * COSVB   +   COSPH * SINVB
      CDPHVB  = COSPH * COSVB   +   SINPH  * SINVB
      SDPHVB  = SINPH * COSVB   -   COSPH * SINVB
   65 IF(ONE23) 70, 70,92
   70 IF(CVB1) 90 , 80,80
   80 IF(COSVB)110,100,100
   90 IF(COSVB)130,120,120
```

```
 92 IF(CVA2) 80,80,90
100 COSA =   CAPHVB * COSGA1 + SAPHVB* SINGA1
    SINA = - SAPHVB * COSGA1 + CAPHVB* SINGA1
    GO TO 140
110 COSA  =-CAPHVB * COSGA1 - SAPHVB * SINGA1
    SINB  =  SAPHVB * COSGA1 - CAPHVB * SINGA1
    GO TO 140
120 COSA  =  CDPHVB * COSGA1 + SDPHVB * SINGA1
    SINA  = -SDPHVB * COSGA1 + CDPHVB * SINGA1
    GO TO 140
130 COSA  =-CDPHVB * COSGA1 - SDPHVB * SINGA1
    SINA  =  SDPHVB * COSGA1 - CDPHVB * SINGA1
140 CAT   =  A2 * SINGA1 * SINA
    CBT   =  COSA/(2.0 * A1)
    SAT   = A2 * SINGA1* COSA
    SBT   =  SINA/(2.0 * A1)
    A12   = A1*A1
    A22   = A2*A2
145 DO 150  I = 1,NR
    XYZ =  (X2(I)*X2(I)*A22 - X1(I)*X1(I)*A12 - PSI(I))/ X1(I)
    COST(I) =   X2(I) *CAT  - XYZ * CBT
150 SINT(I) =   X2(I) * SAT  + XYZ * SBT
    GO TO  270
160 IF(1.0-ABSF(COSVA))162,162,163
162 SINVA=0.0
    GO TO 164
163  SINVA = SQRTF( 1.0 - COSVA*COSVA)
164 CAPHVA = COSPH * COSVA  -  SINPH* SINVA
    SAPHVA = SINPH * COSVA  +  COSPH * SINVA
    CDPHVA = COSPH * COSVA  +  SINPH * SINVA
    SDPHVA = SINPH * COSVA  -  COSPH * SINVA
165 IF(ONE23) 170,200,170
170 IF(CVA1) 190,180,180
180 IF(COSVA) 220,210,210
190 IF(COSVA) 240,230,230
200 IF(CVA2) 190,180,180
210 COSA =  CAPHVA * COSGA1 -  SAPHVA * SINGA1
    SINA =  SAPHVA * COSGA1 +  CAPHVA * SINGA1
    GO TO 250
220 COSA  = - CAPHVA * COSGA1 + SAPHVA * SINGA1
    SINA  = - SAPHVA * COSGA1 - CAPHVA * SINGA1
    GO TO 250
230 COSA  = CDPHVA * COSGA1 - SDPHVA * SINGA1
    SINA  = SDPHVA * COSGA1 + CDPHVA * SINGA1
    GO TO 250
240 COSA =  - CDPHVA * COSGA1 + SDPHVA * SINGA1
    SINA =  - SDPHVA * COSGA1 - CDPHVA * SINGA1
250  CAT =  A1*SINGA1*SINA
     CBT  = COSA/(2.0* A2)
     SAT =  A1 * SINGA1 * COSA
     SBT =  SINA/( 2.0* A2)
     A12 = A1*A1
     A22 = A2*A2
255 DO 260  I = 1, NR
```

```
    XYZ = (X1(I)*X1(I) * A12 -  X2(I)* X2(I) * A22 - PSI(I))/ X2(I)
    COST(I) =  X1(I) * CAT  -  XYZ * CBT
260 SINT(I) =  X1(I) * SAT  +  XYZ * SBT
270  SINU = SINF(UM)
     COSU = COSF(UM)
    TAN2U =(SINU/COSU)**2
     SUCU = SINU*COSU
    IF(ZETA)271,272,272
271 ZETA=0.0
272  ETAA = SINU*SINU - 1.0 +(COSU -SQRTF(ZETA))**2
     ETAB =  2.0* SINU
     YAMB = (1.0/(2.0 * YAM))**2
275 DO 280  I =1,NR
    COSETA  = (PSI(I) + ETAA)/ ETAB
    CO2ETA  = COSETA * COSETA
    SI2ETA  =PSI(I)    -CO2ETA
    IF(SI2ETA)276,276,277
276 SINETA=0.0
    REJQ(I)=REJQ(I) + 10.0
    GO TO 278
277 SINETA  = SQRTF(SI2ETA)
278 ABC  =   CO2ETA * SINT(I)* SINT(I)  + SI2ETA *COST(I)* COST(I)
    DEF  =  2.0* SINETA*COSETA * SINT(I)* COST(I)
    PL(I)=  SINETA * SUCU /(4.0 +( 2.0 - (PSI(I)+ ZETA)*(PSI(I)+ZETA))
   1     )/ ( 1.0/ (1.0 + TAN2U*(ABC + DEF      )/(PSI(I)*PSI(I)))
   1         +1.0/ (1.0 + TAN2U*(ABC - DEF      )/(PSI(I)*PSI(I))))
   1 *50.
    AVEQ(I) = AVEQ(I) * PL(I)
    PL(I)  =  SQRTF(PL(I))
    SI(I)=(PSI(I)+ZETA)*YAMB
    IF(SINH-SI(I))279,279,280
279 AVEQ(I)=AVEQ(I)*1.5
280 CONTINUE
    RETURN
    END(1,1,0,0,0)
```

```
      SUBROUTINE WESSLP( YAM,NR,R1,R2,SINH,     ZETA,BSE)
      DIMENSION AVEQ(1000),PSI(1000),PL(1000),SI(1000),H1(1000),
     1 H2(1000),H3(1000),EPS(1000),REJQ(1000),RENO(1000)
      COMMON H1,H2,H3,EPS,AVEQ,REJQ,RENO
      COMMON PSI,PL,SI
      FREQUENCY 90(250),105(0,4,1),120(2,2,1),130(250),150(250)
     1,91(1,1,100),135(100,10,1),155(100,10,1),141(100,1,1)
      YAMB =(1.0/(2.0 * YAM))**2
   90 DO 100  I = 1,NR
   91 IF(4.0- PSI(I)-ZETA) 92,92,93
   92 REJQ(I) = REJQ(I) + 10.0
      PL(I) = 0.0
      GO TO 94
   93 PL(I) = 2.0* SQRTF(PSI(I)*(4.0-PSI(I) - ZETA))/
     1          (4.0  + (2.0 - PSI(I) - ZETA)*(2.0 - PSI(I) - ZETA))
   94 AVEQ(I) = AVEQ(I) * PL(I)
      PL(I) = SQRTF(PL(I))
      SI(I) =       (PSI(I) + ZETA) * YAMB
      IF(SINH-SI(I))95,95,100
   95 AVEQ(I)=AVEQ(I)*1.5
  100 CONTINUE
  105 IF(ZETA-1.0E-10)170,170,110
  110 PSIM = 4.0 - ZETA
      RZ  =  180.0 * SQRTF(ZETA)/(12.56636 *(2.0 * R1/SQRTF(PSIM) +R2))
  120 IF(BSE)150,170,130
  130 DO 145I = 1,NR
  135 IF(REJQ(I)-10.0)140,145,145
  140 YDEL  = RZ * SQRTF(PSIM/PSI(I) - 1.0)
  141 IF(1.0-YDEL-1.0E-02)142,142,143
  142 AVEQ(I)=0.0
      REJQ(I)=REJQ(I)+20.0
      GO TO 145
  143 AVEQ(I) = AVEQ(I) * (1.0- YDEL)
      PL(I)=PL(I)*SQRTF(1.0-YDEL)
  145 CONTINUE
      GO TO 170
  150 DO 165 I = 1,NR
  155 IF(REJQ(I)-10.0)160,165,165
  160 YDEL  = RZ * SQRTF(PSIM/PSI(I) -1.0)
      AVEQ(I) = AVEQ(I) * (1.0 + YDEL)
      PL(I)=PL(I)*SQRTF(1.0+YDEL)
  165 CONTINUE
  170 RETURN
      END(2,2,2,2,2)
```

```
      SUBROUTINE DICORD(U1,U2,U3,CE,PE,SL,NR,TL)
      DIMENSION H1(1000),H2(1000),H3(1000),EPS(1000),AVEQ(1000),
     1REJQ(1000),RENO(1000),PL(1000),SI(1000),PSI(1000)
      COMMON H1,H2,H3,EPS,AVEQ,REJQ,RENO
      COMMON PSI,PL,SI
      WRITE TAPE 7,U1,U2,U3,CE,PE
      WRITE TAPE 7,SL,NR,TL
      WRITE TAPE 7,(H1(I),H2(I),H3(I),EPS(I),AVEQ(I),REJQ(I),RENO(I),
     1PL(I),SI(I),I=1,NR)
      RETURN
      END(0,1,0,0,0)
```

```
      SUBROUTINE REJECT(NS)
      DIMENSION H1(1000),H2(1000),H3(1000),AVEQ(1000),REJQ(1000),PL(1000
     1),SI(1000),SPE(1000),PSE(1000),ESP(1000)
      COMMON H1,H2,H3,SPE,AVEQ,REJQ,PSE,ESP,PL,SI
      FREQUENCY 5(20),10(250),20(0,20,1)
      REWIND 7
      IF(SENSESWITCH 6)2,3
    2 PRINT 500
      PRINT 560
    3 WRITE OUTPUT TAPE 9,500
      WRITE OUTPUT TAPE 9, 560
    5 DO 50 J=1,NS
      READ TAPE 7,U1,U2,U3,CE,PE
      READ TAPE 7,SL,NR,TL
      READ TAPE 7,(H1(I),H2(I),H3(I),EPS,AVEQ(I),REJQ(I),EPS,PL(I),
     1 SI(I),I=1,NR)
      MSL=INTG(SL)
      MU1=INTG(U1)
      MU2=INTG(U2)
      MU3=INTG(U3)
      IF(SENSESWITCH 6)6,7
    6 PRINT 560
      PRINT 670,MU1,MU2,MU3,MSL
    7 WRITE OUTPUT TAPE 9,560
      WRITE OUTPUT TAPE 9, 670,MU1,MU2,MU3,MSL
   10 DO 40 I=1,NR
   20 IF(REJQ(I))   40,40,30
   30 MH1=INTG(H1(I))
      MH2=INTG(H2(I))
      MH3=INTG(H3(I))
      MRJ=INTG(REJQ(I))
      IF(SENSESWITCH 6)32,33
   32 PRINT 510,MH1,MH2,MH3,SI(I),PL(I),AVEQ(I),MRJ
   33 WRITE OUTPUT TAPE 9, 510,MH1,MH2,MH3,SI(I),PL(I),AVEQ(I),MRJ
   40 CONTINUE
   50 CONTINUE
      REWIND 7
      RETURN
  500 FORMAT(1H1,84H      H    K    L             SIN()/L          LP FACTOR
     1            F**2                R)
  560 FORMAT(1H0)
  670 FORMAT(1H0,3I3,9H    LAYERI3)
  510 FORMAT(1H0,2H  3I4,F19.7,F18.6,F19.3,I14)
      END(2,2,2,2,2)
```

```
      SUBROUTINE LSQCOR(NS)
      DIMENSION H1(1000),H2(1000),H3(1000),REJQ(1000),AVEQ(1000),
     1G1(1000),G2(1000),G3(1000),AVEQ1(1000),REJQ1(1000),RENO1(1000),
     2C(50),A(50,50),M4(100),M5(100),M6(100),TRENO(100),TAVEQ(100),
     3N4(100),N5(100),N6(100),TAVEQ1(100),TRENO1(100),X(50),
     4RENO(1000),EPS(1000),PL(1000),SI(1000),B(50)
      COMMON H1,H2,H3,EPS,AVEQ,REJQ,RENO
      COMMON M4,M5,X,C,TRENO,TAVEQ,N4,N5,N6,M6,TAVEQ1
      COMMON PL,SI,G1,G2,G3,AVEQ1,REJQ1,RENO1,A,B,TRENO1
      FREQUENCY   270(20),292(0,1,1),295(0,6,1),320(30,1,30),
     1330(0,1,10),331(0,5,1),315(300),355(30,1,30),360(0,1,10),
     2361(0,5,1),350(300),375(1,2,1),410(1,15,1),420(1,9,1),430(1,5,1),
     3460(1,1,4),470(1,1,4),471(1,1,4),472(1,1,4),491(0,6,1),495(0,2,1),
     4526(300)
      REWIND 6
      REWIND 7
      REWIND 8
      DO 200 I=1,NS
  200 A(I,I)=0.0
      JK=1
      N1=3*NS-3
      READ TAPE 7,U1,U2,U3,CE,PE
      IF(CE) 20,20,201
  201 DO 202 I=1,NS
  202 X(I) =1.0
      REWIND 7
      GO TO 525
  265 JK = JK + 1
  270 DO  280  I= 1,N1
  280 BACK SPACE 7
      N1 = N1 - 3
  290 READ TAPE 7, U1,U2,U3,CE,PE
   20 READ TAPE 7, SL,NR,TL
      READ TAPE 7,(H1(I),H2(I),H3(I), PS, AVEQ(I),REJQ(I),RENO(I),
     1 PS, PS,I = 1,NR)
  292 IF(CE)291,291,500
  291 N = JK
  295 IF(TL) 300,300,310
  300 READ TAPE 7, V1,V2,V3,CE1,PE1
      READ TAPE 7, SL1,NR1,TL
      READ TAPE 7,(G1(I),G2(I),G3(I), PS, AVEQ1(I),REJQ1(I),RENO1(I),
     1 PS, PS,I =1,NR1)
      N = N +1
      A(JK,N)=0.0
      A(N,JK)=0.0
      GO TO 295
  310 READ TAPE 7, V1,V2,V3,CE1,PE1
      READ TAPE 7, SL1,NR1,TL
      READ TAPE 7,(G1(I),G2(I),G3(I), PS, AVEQ1(I),REJQ1(I),RENO1(I),
     1 PS, PS,I =1,NR1)
      N = N + 1
      IF(U1-V1)314,311,314
  311 IF(U2-V2)314,312,314
  312 IF(U3-V3)314,313,314
```

```
313 A(JK,N)=0.0
    A(N,JK)=0.0
    GO TO 491
314 SRENO = 0.0
    SAVEQ = 0.0
    SAVEQ1= 0.0
    J1 = 0
315 DO 340 I = 1,NR
320 IF(ABSF(SL1-ABSF(V1*H1(I)+V2*H2(I)+V3*H3(I)))-1.0E-05)330,330,340
330 IF(AVEQ(I))331,331,332
331 IF(REJQ(I))332,332,340
332 J1 = J1 + 1
    M4(J1)=INTG(H1(I))
    M5(J1)=INTG(H2(I))
    M6(J1)=INTG(H3(I))
    TRENO(J1) = RENO(I)
    TAVEQ(J1) = AVEQ(I)
340 CONTINUE
    J2 = 0
350 DO 370 I  = 1,NR1
355 IF(ABSF(SL -ABSF(U1*G1(I)+U2*G2(I)+U3*G3(I)))-1.0E-05)360,360,370
360 IF(AVEQ1(I))361,361,362
361 IF(REJQ1(I))362,362,370
362 J2 = J2 + 1
    N4(J2)=INTG(G1(I))
    N5(J2)=INTG(G2(I))
    N6(J2)=INTG(G3(I))
    TRENO1(J2)= RENO1(I)
    TAVEQ1(J2)= AVEQ1(I)
370 CONTINUE
    L = 0
    M = 0
375 IF(J1 - J2) 390,390,380
380  J  =  J2
    JB=J1
    GO TO 400
390  J = J1
    JB=J2
400  DO  485     I = 1,J
405 IL=I+L
    IM=I+M
410 IF(M4(IL)-N4(IM))440,420,450
420 IF(M5(IL)-N5(IM))440,430,450
430 IF(M6(IL)-N6(IM))440,471,450
440 L = L + 1
    GO TO 460
450 M = M + 1
460 IF(JB-IL    )490,470,470
470 IF(JB-IM    )490,405,405
471 IF(JB-IL)490,472,472
472 IF(JB-IM)490,480,480
480 SRENO = SRENO + TRENO(IL ) + TRENO1(IM   )
    SAVEQ = SAVEQ + (TRENO(IL ) + TRENO1(IM ))* TAVEQ(IL )/
   1(TAVEQ(IL ) + TAVEQ1(IM ))
```

```
485 SAVEQ1 =  SAVEQ1 + (TRENO(IL ) + TRENO1(IM ))* TAVEQ1(IM )/
   1(TAVEQ(IL ) + TAVEQ1(IM ))
490  A(JK,JK) = A(JK,JK) + SAVEQ * SAVEQ / SRENO
     A(N,N) =  A(N,N) +  SAVEQ1 * SAVEQ1 / SRENO
     A(JK,N) = - SAVEQ * SAVEQ1 / SRENO
     A(N,JK) = A(JK,N)
491 IF(TL) 310,310, 495
495 IF(CE1)310,310, 265
500 REWIND 7
    SN=NS
    AVA=0.0
    DO 501 I=1,NS
501 AVA=AVA+A(I,I)
    AVA=AVA/SN
    DO 502 I=1,NS
    DO 502 J=1,NS
502 A(I,J)=A(I,J)/AVA
    WRITE TAPE 6,((A(I,J),I=1,NS),J=1,NS)
    REWIND 6
    CALL EIGEN(A,C,NS)
    SMC=C(1)
    DO 513 I=2,NS
    IF(C(I)-SMC)512,513,513
512 SMC=C(I)
513 CONTINUE
    READ TAPE 6,((A(I,J),I=1,NS),J=1,NS)
    REWIND 6
    CALL VCTR(A,X,NS,SMC)
525 DO  540   I = 1,NS
    READ TAPE 7, V1,V2,V3,CE1,PE1
    READ TAPE 7, SL ,NR ,TL
    READ TAPE 7,(H1(J),H2(J),H3(J),EPS(J),AVEQ(J),REJQ(J),RENO(J),
   1PL(J),SI(J),J=1,NR)
526 DO  530   J  = 1,NR
530 AVEQ(J) = X(I)    * AVEQ(J)
    WRITE TAPE 6,V1,V2,V3,CE1,PE1
    WRITE TAPE 6,SL,NR,TL
    WRITE TAPE 6,(H1(J),H2(J),H3(J),EPS(J),AVEQ(J),REJQ(J),RENO(J),
   1PL(J),SI(J),J=1,NR)
    WRITE TAPE 8,V1,V2,V3,CE1,PE1
    WRITE TAPE 8,SL,NR,TL
540 WRITE TAPE 8,(H1(J),H2(J),H3(J),EPS(J),AVEQ(J),REJQ(J),RENO(J),
   1PL(J),SI(J),J=1,NR)
545 REWIND 6
    REWIND 7
    REWIND 8
    RETURN
    END(0,1,0,0,0)
```

```
      SUBROUTINE IAVOR(NS,NOZ)
      DIMENSION H1(1000),H2(1000),H3(1000),EPS(1000),AVEQ(1000),REJQ(100
     1 0),RENO(1000),SI(1000),H1L(50),H1H(50),F1(1000),F2(1000),F3(1000)
     1 ,FAVEQ(1000),FRENO(1000),FEPS(1000),FREJQ(1000),FSI(1000),FH1(100
     1 ),FH2(100),FH3(100),GAVEQ(100),GRENO(100),GEPS(100),GREJQ(100),
     1 GSI(100),FG1(100),FG2(100),FG3(100),HEPS(100),HAVEQ(100),
     1HRENO(100),HREJQ(100),HSI(100),X(50,1)
      FREQUENCY 290(0,1,5),305(9),540(9),545(2,1,7),565(9),566(2,1,7),
     1 595(9),597(5,1,5),605(5,1,5),635(0,0,1),655(300),657(2,1,7),
     1 675(300),677(2,1,7),696(300),697(5,1,5),712(0,0,1),716(50),717(
     1 2,1,7),735(50),737(2,1,7),755(25),756(50),757(5,1,5),822(0,1,10),
     1 827(0,1,7),600(300),792(0,1,3)
      COMMON H1,H2,H3,EPS,AVEQ,REJQ,RENO
      COMMON FH1,FH2,X,H1H,FH3,GAVEQ,GRENO,GEPS,GREJQ,GSI,FG1
      COMMON F1,SI,F2,F3,FAVEQ,FRENO,FEPS,FREJQ,FSI
      COMMON FG3,HEPS,HAVEQ,HRENO,HREJQ,H1L,FG2,HSI
      NOZ = 0
  300 READ TAPE 7, V1,V2,V3,CE,PE
      READ TAPE 7 ,SL,NR,TL
      READ TAPE 7 ,( H1(I),EP ,EP,EP,EP,EP,EP,EP,EP, I = 1,NR)
      H1L(1) = H1(1)
      H1H(1) = H1(NR)
      IF(NS-1)315,315,305
  305 DO 310  J = 2,NS
      READ TAPE 7 , V1,V2,V3,CE,PE
      READ TAPE 7 , SL,NR,TL
      READ TAPE 7 ,( H1(I),EP,EP,EP,EP,EP,EP,EP,EP,I = 1,NR)
      H1L(J) = H1(1)
  310 H1H(J) = H1(NR)
  315 REWIND 7
      SMH1 = H1L(1)
  540 DO  560  I = 1,NS
  545 IF(H1L(I) - SMH1) 550,560,560
  550 SMH1 =  H1L(I)
  560 CONTINUE
      MH1=INTG(SMH1)
      BIGH1 = H1H(1)
  565 DO  580   I = 1,NS
  566 IF(BIGH1 - H1H(I))570,580,580
  570 BIGH1 = H1H(I)
  580 CONTINUE
      IGH1=INTG(BIGH1)
      IJ=1
  590 L=0
      IF(IJ/2)100,100,110
  100 IJ=2
      GO TO 595
  110 IJ=1
  595 DO 630 I=1,NS
      GO TO(596,598),IJ
  596 READ TAPE 6 , V1,V2,V3,CE, PE
      READ TAPE 6 , SL,NR,TL
      READ TAPE 6,( H1(I),H2(I),H3(I),EPS(I),AVEQ(I),REJQ(I),RENO(I),
     1                      PL ,SI(I), I = 1,NR)
```

```
    GO TO 597
598 READ TAPE 8 , V1,V2,V3,CE, PE
    READ TAPE 8 , SL,NR,TL
    READ TAPE 8,( H1(I),H2(I),H3(I),EPS(I),AVEQ(I),REJQ(I),RENO(I),
   1                   PL ,SI(I), I = 1,NR)
597 IF(INTG(H1(1))-MH1)600,600,630
600 DO  620    J = 1,NR
605 IF(INTG(H1(J))-MH1)620,610,630
610 L = L + 1
    F1(L) = H1(J)
    F2(L) = H2(J)
    F3(L) = H3(J)
    FAVEQ(L) = AVEQ(J)
    FRENO(L) = RENO(J)
    FEPS(L)  = EPS(J)
    FREJQ(L) =  REJQ(J)
    FSI(L)   =  SI(J)
620 CONTINUE
630 CONTINUE
    REWIND 6
    REWIND 8
635 IF(L)825,825,650
650 SMH2 = F2(1)
655 DO 670  I =1,L
657 IF(F2(I) - SMH2)660,670,670
660 SMH2  = F2(I)
670 CONTINUE
    MH2=INTG(SMH2)
    BIGH2 = F2(1)
675 DO 690  I =1,L
677 IF(BIGH2 - F2(I))680,690,690
680 BIGH2 = F2(I)
690 CONTINUE
    IGH2=INTG(BIGH2)
695 L1 =  0
696 DO 710  I = 1,L
697 IF(INTG(F2(I))-MH2)710,700,710
700 L1 = L1 + 1
    FH1(L1) = F1(I)
    FH2(L1) = F2(I)
    FH3(L1) = F3(I)
    GAVEQ(L1) = FAVEQ(I)
    GRENO(L1) = FRENO(I)
    GEPS(L1)  = FEPS(I)
    GREJQ(L1) = FREJQ(I)
    GSI(L1) =  FSI(I)
710 CONTINUE
712 IF(L1)820,820,715
715 SMH3 = FH3(1)
716 DO 730  I = 1,L1
717 IF(FH3(I) - SMH3) 720,730,730
720 SMH3 = FH3(I)
730 CONTINUE
    MH3=INTG(SMH3)
```

```
    BIGH3 = FH3(1)
735 DO  750  I = 1,L1
737 IF(BIGH3 - FH3(I)) 740,750,750
740 BIGH3 = FH3(I)
750 CONTINUE
    IGH3=INTG(BIGH3)
    IBIG=0
     MH3 =  MH3 - 1
    JBIG= IGH3- MH3
755 DO 800 I  = 1,JBIG
     MH3  =   MH3 + 1
    L2=0
    ZIP=0.0
    ZAP=0.0
    ZOP=0.0
756 DO 790  J = 1,L1
757 IF(MH3-INTG(FH3(J)))790,760,790
760 L2=1
    WIP=FH1(J)
    WAP=FH2(J)
    WOP=FH3(J)
    WUP=GEPS(J)
    ZIP=ZIP+GRENO(J)*GAVEQ(J)
    ZAP=ZAP+GRENO(J)
    ZOP=ZOP+GREJQ(J)
    ZUP=GSI(J)
790 CONTINUE
792 IF(L2)800,800,795
795 IBIG=IBIG+1
    FG1(IBIG)=WIP
    FG2(IBIG)=WAP
    FG3(IBIG)=WOP
    HAVEQ(IBIG)=ZIP/ZAP
    HREJQ(IBIG)=ZOP
    HSI(IBIG)=ZUP
    HEPS(IBIG)=WUP
    HRENO(IBIG)=ZAP
800 CONTINUE
810 NOZ = NOZ + 1
    WRITE TAPE 7, IBIG
    WRITE TAPE 7,( FG1(I),FG2(I),FG3(I),HAVEQ(I),HEPS(I),HREJQ(I),
   1 HRENO(I),                HSI(I), I = 1,IBIG)
820  MH2 =  MH2  + 1
822 IF( IGH2 -  MH2)825,695,695
825  MH1 =  MH1  +1
827 IF( IGH1 -  MH1)830,590,590
830 REWIND 7
    REWIND 6
    REWIND 8
    RETURN
    END(0,1,0,0,0)
```

```
      SUBROUTINE ABSI (SYAM,AS,BS,CS,AS1,BS1,NASP,AN,S2I,NOZ,EX,SF,NI,
     1 BT1,BT2)
      DIMENSION  SXT(100),SIG(100),YSN(100),YSD(100),WI(100),AVEQ(1000),
     1      EPS(1000), REJQ(1000),SI(1000),YST(100),AN(20),AS(20),
     1      AS1(20),BS(20),BS1(20),CS(20),H1(1000),H2(1000),H3(1000),
     1 RENO(1000),ZXY(350),X(50,1),PL(1000),TXT(100),AT1(19),AT2(19)
     1 ,SAG(19)
      COMMON H1,H2,H3,EPS,AVEQ,REJQ,RENO
      COMMON SXT,YST,X,WI ,YSN,YSD,SIG,ZXY,PL,SI ,TXT,AT1,AT2,SAG
      FREQUENCY 10(40),20(4),32(40),40(15),47(300),60(40),100(40),
     1 115(15),117(300),48(0,15,1),50(0,1,10),65(20,1,4)
      SIMAX  = (1.0/SYAM ) ** 2
      NI  =XINTF( SIMAX/S2I)
      SXT(1)=   S2I / 2.0
   10 DO  30    I = 2,NI
   30 SXT(I)= SXT(I-1) + S2I
      DO  31 I=1,NI
      SIG(I) = 0.0
   20 DO  31    J = 1,NASP
   31 SIG(I) = SIG(I) +  AN(J)*( AS(J)*EXPF(-AS1(J)*SXT(I))+
     1               BS(J)*EXPF(- BS1(J)*SXT(I)) + CS(J))**2
   32 DO  35    I =1,NI
      YSN(I) = 0.0
      YSD(I) = 0.0
   35 WI(I) = 0.0
   40 DO   95  NIP = 1,NOZ
   45 READ TAPE 7, IBIG
      READ TAPE 7,(AB1,BB1,CB1,       AVEQ(I),EPS(I),REJQ(I),RENO(I),
     1 SI(I),      I = 1,IBIG)
   47 DO  90      I = 1,IBIG
      SIX = 0.0
   50 IF(AVEQ(I))48,48,60
   48 IF(REJQ(I))60,60,90
   60 DO  80    J = 1,NI
      SIX = SIX + S2I
   65 IF(SIX - SI(I)) 80, 70,70
   70  YSN(J) = EPS(I) * SIG(J)   + YSN(J)
       YSD(J) = YSD(J) + AVEQ(I)
       WI(J)  = WI(J) + 1.0
      GO TO 90
   80  CONTINUE
   90 CONTINUE
   95 CONTINUE
      REWIND 7
      DO 98 I=1,NI
      IF(YSD(I)-1.0E-10)96,96,97
   96 YST(I)=0.0
      GO TO 98
   97 YST(I) = LOGF( YSN(I)/ YSD(I))
   98 CONTINUE
      EX=.5
      DO 111 J=1,19
      WXX = 0.0
      WY = 0.0
```

```
      WX = 0.0
      WXY =0.0
      WT = 0.0
      EX=EX+.5
  100 DO  110  I = 1,NI
      TXT(I)=SXT(I)**EX
      WT =  WT + WI(I)
      WXX = WXX +  WI(I) * TXT(I) * TXT(I)
      WY  = WY  +  WI(I) * YST(I)
      WX = WX + WI(I) * TXT(I)
      WXY = WXY + WI(I) * TXT(I) * YST(I)
  110 CONTINUE
      AT1(J)=( WT* WXY  - WX * WY )/(WT * WXX  -WX**2)
      AT2(J)=(WY-AT1(J)*WX)/WT
      SAG(J)=0.0
      DO 1111I=1,NI
      IF(YSD(I)-1.0E-10)1111,1111,1110
 1110 SAG(J)=SAG(J)+(AT2(J)+AT1(J)*TXT(I)-YST(I))**2
 1111 CONTINUE
  111 CONTINUE
      SSAG=SAG(1)
      DO 113 I=1,19
      IF(SAG(I)-1.0E-10)113,113,12
   12 IF(SSAG-SAG(I))113,112,112
  112 BT1=AT1(I)
      BT2=AT2(I)
      EX=0.5+0.5*FLOATF(I)
      SSAG=SAG(I)
  113 CONTINUE
      SF =  EXPF(BT2)
  115 DO 120  J =1, NOZ
      READ TAPE 7 ,  IBIG
      READ TAPE 7 ,(H1(I),H2(I),H3(I),AVEQ(I),EPS(I),REJQ(I),RENO(I),
     1 SI(I),      I = 1,IBIG)
  117 DO 130  I = 1,IBIG
  130 AVEQ(I) =  AVEQ(I) * SF
      WRITE TAPE 8, IBIG
  120 WRITE TAPE 8,(H1(I),H2(I),H3(I),AVEQ(I),EPS(I),REJQ(I),RENO(I),
     1 SI(I),      I = 1,IBIG)
      REWIND 7
      REWIND 8
      RETURN
      END(2,2,2,2,2)
```

```
      SUBROUTINE OUTPUT(NOZ,NS,NI,BT1,BT2,SF,EX,NOIB)
      DIMENSION H1(1000),H2(1000),H3(1000),AVEQ(1000),EPS(1000),REJQ
     1(1000),RENO(1000),PL(1000),SI(1000),RAVEQ(1000),WEI(1000),Y1(50),
     2Y2(50),Y3(50),M1(1000),M2(1000),M3(1000),YAVEQ(50),YRAVEQ(50),
     3MRENO(1000),YWEI(50),MREJQ(1000),MEPS(1000),SXT(100),YST(100),
     4X(50),  BCB(450),YSI(50),WI(100)
      COMMONH1,H2,H3,EPS,AVEQ,REJQ,RENO,SXT,YST,X,WI,    Y3,YAVEQ,YRAVEQ
     1,YWEI,BCB,PL,SI,RAVEQ,WEI,M1,M2,M3,MREJQ,MRENO,MEPS,Y1,Y2
      FREQUENCY 190(15),195(25),260(0,1,10),300(50,1,0),340(0,1,20),
     1362(5),363(300),390(0,1,10),435(0,3,1),440(0,1,3),805(5,1,30),
     2480(2,1,15)
      QN=1.0
      N=0
      NOIB=0
      NNN=1
  190 DO 330 J=1,NOZ
      READ TAPE 8,IBIG
      READ TAPE 8,(H1(I),H2(I),H3(I),AVEQ(I),EPS(I),REJQ(I),RENO(I),
     1SI(I),I=1,IBIG)
      NOIB=NOIB+IBIG
  195 DO 320 I=1,IBIG
  220 RAVEQ(I)=SQRTF(AVEQ(I))
      SI(I)=SQRTF(SI(I))
  260 IF(RENO(I))270,270,280
  270 WEI(I)=0.0
      GO TO 290
  280 WEI(I)=RAVEQ(I)/SQRTF(RENO(I))
  290 N=N+1
      Y1(N)=H1(I)
      Y2(N)=H2(I)
      Y3(N)=H3(I)
      M1(N)=INTG(H1(I))
      M2(N)=INTG(H2(I))
      M3(N)=INTG(H3(I))
  299 YSI(N)=SI(I)
      YAVEQ(N)=AVEQ(I)
      YRAVEQ(N)=RAVEQ(I)
      MRENO(N)=RENO(I)+.0001
      YWEI(N)=WEI(I)
      MREJQ(N)=INTG(REJQ(I))
      MEPS(N)=INTG(EPS(I))
  300 IF(N-25)320,310,310
  310 IF(SENSESWITCH 6)311,312
  311 PRINT 540
      PRINT 600
      PRINT 560,(M1(K),M2(K),M3(K),YSI(K),YAVEQ(K),YRAVEQ(K),MEPS(K),
     1MRENO(K),MREJQ(K),K=1,25)
  312 WRITE OUTPUT TAPE 9, 540
      WRITE OUTPUT TAPE 9,600
      WRITE OUTPUT TAPE 9, 560, (M1(K),M2(K),M3(K),YSI(K),YAVEQ(K),YRAVE
     1Q(K),MEPS(K),MRENO(K),MREJQ(K),K=1,25)
      WRITE OUTPUT TAPE 5,580,(Y1(K),Y2(K),Y3(K), YAVEQ(K),YWEI(K),QN,
     1YSI(K),K=1,N)
      N=0
```

```
320 CONTINUE
330 CONTINUE
340 IF(N)360,360,350
350 IF(SENSESWITCH 6)351,352
351 PRINT 540
    PRINT 550
    PRINT 560,(M1(K),M2(K),M3(K),YSI(K),YAVEQ(K),YRAVEQ(K),MEPS(K),
   1MRENO(K),MREJQ(K),K=1,N)
352 WRITE OUTPUT TAPE 9,540
    WRITE OUTPUT TAPE 9,550
    WRITE OUTPUT TAPE 9,560,(M1(K),M2(K),M3(K),YSI(K),YAVEQ(K) ,YRAVEQ
   1(K),MEPS(K),MRENO(K),MREJQ(K),K=1,N)
    WRITE OUTPUT TAPE 5,580,(Y1(K),Y2(K),Y3(K), YAVEQ(K),YWEI(K),QN,
   1YSI(K),K=1,N)
360 END FILE 5
    REWIND 5
    REWIND 8
    IF(SENSESWITCH 6)353,361
353 PRINT 600
    PRINT 690,NOIB
    PRINT 530
    PRINT 590,BT2,BT1,EX,SF
    PRINT 600
    PRINT 610
    PRINT 550
    PRINT 620,(SXT(K),YST(K),WI(K),K=1,NI)
361 WRITE OUTPUT TAPE 9,600
    WRITE OUTPUT TAPE 9,690,NOIB
    WRITE OUTPUT TAPE 9,530
    WRITE OUTPUT TAPE 9,590,BT2,BT1,EX,SF
    WRITE OUTPUT TAPE 9,600
    WRITE OUTPUT TAPE 9,610
    WRITE OUTPUT TAPE 9,550
    WRITE OUTPUT TAPE 9,620,(SXT(K),YST(K),WI(K),K=1,NI)
362 DO 820 K=1,NS
    READ TAPE 6,U1,U2,U3,CE,PE
    READ TAPE 6,SL,NR,TL
    READ TAPE 6,(H1(J),H2(J),H3(J),EPS(J),AVEQ(J),REJQ(J),RENO(J),
   1PL(J),SI(J),J=1,NR)
    MU1=INTG(U1)
    MU2=INTG(U2)
    MU3=INTG(U3)
    MSL=INTG(SL)
363 DO 430 I=1,NR
    AVEQ(I)=AVEQ(I)*SF
    RAVEQ(I)=SQRTF(AVEQ(I))
    SI(I)=SQRTF(SI(I))
390 IF(RENO(I))400,400,410
400 WEI(I)=0.0
    GO TO 420
410 WEI(I)=RAVEQ(I)/SQRTF(RENO(I))
420 M1(I)=INTG(H1(I))
    M2(I)=INTG(H2(I))
    M3(I)=INTG(H3(I))
```

```
      MREJQ(I)=INTG(REJQ(I))
      MRENO(I)=INTG(RENO(I))
  430 MEPS(I)=INTG(EPS(I))
      NR1=NR
  435 IF(PE)437,437,436
  436 IF(SENSESWITCH 6)10,20
   10 PRINT 635
   20 WRITE OUTPUT TAPE 9,635
      GO TO 440
  437 IF(SENSESWITCH 6)30,40
   30 PRINT 630
   40 WRITE OUTPUT TAPE 9,630
      GO TO(440,450,465),NNN
  440 IF(CE)460,460,445
  445 NNN=2
  450 IF(SENSESWITCH 6)   50,60
   50 PRINT 640,MU1,MU2,MU3,MSL,SF,NR
   60 WRITE OUTPUT TAPE 9,640 ,MU1,MU2,MU3,MSL,SF,NR
      GO TO 470
  460 NNN=3
  465 X(K)=X(K)*SF
      IF(SENSESWITCH 6)466,467
  466 PRINT 640,MU1,MU2,MU3,MSL,X(K),NR
  467 WRITE OUTPUT TAPE 9,640,MU1,MU2,MU3,MSL,X(K),NR
  470 IF(SENSESWITCH 6)471,472
  471 PRINT 550
      PRINT 650
      PRINT 600
  472 WRITE OUTPUT TAPE 9, 550
      WRITE OUTPUT TAPE 9,650
      WRITE OUTPUT TAPE 9,600
  480 IF(NR1-22)490,490,800
  490 NR2=NR-NR1+1
      IF(SENSESWITCH 6) 491,492
  491 PRINT 660,(M1(I),M2(I),M3(I),SI(I),PL(I),AVEQ(I),RAVEQ(I),MEPS
     1(I),MRENO(I),MREJQ(I),I=NR2,NR)
  492 WRITE OUTPUT TAPE 9,660,(M1(I),M2(I),M3(I),SI(I),PL(I),AVEQ(I),RAV
     1EQ(I),MEPS(I),MRENO(I),MREJQ(I),I=NR2,NR)
      GO TO 810
  800 NR2=NR-NR1+1
      NR3=NR2+23
      IF(SENSESWITCH 6)801,802
  801 PRINT 660,(M1(I),M2(I),M3(I),SI(I),PL(I),AVEQ(I),RAVEQ(I),MEPS
     1(I),MRENO(I),MREJQ(I),I=NR2,NR3)
  802 WRITE OUTPUT TAPE 9,660,(M1(I),M2(I),M3(I),SI(I),PL(I),AVEQ(I),RAV
     1EQ(I),MEPS(I),MRENO(I),MREJQ(I),I=NR2,NR3)
      NR1=NR1-24
      IF(SENSESWITCH 6)803,804
  803 PRINT 670 ,MU1,MU2,MU3,MSL
      PRINT 650
      PRINT 600
  804 WRITE OUTPUT TAPE 9,670,MU1,MU2,MU8,MSL
      WRITE OUTPUT TAPE 9,650
      WRITE OUTPUT TAPE 9,600
```

```
805 IF(NR1-24)490,490,800
810 WRITE OUTPUT TAPE 7,580,H1(1),H2(1),H3(1), AVEQ(1),WEI(1),QN,SI(1)
    WRITE OUTPUT TAPE 7,680,(H1(I),H2(I),H3(I), AVEQ(I),WEI(I), SI(I),
   1I=2,NR)
820 CONTINUE
    END FILE 7
    REWIND 6
    REWIND 7
    RETURN
540 FORMAT(1H1,106H                H    K    L              SIN()/L
   1    F**2              F                EPS        W         R)
550 FORMAT(1H )
560 FORMAT(1H0,12H           3I4,F18.7,F19.3,F18.4,3I9)
530 FORMAT(1H1)
580 FORMAT(6F9.2,F9.6,9H        R,12X)
590 FORMAT(33H  LOG K = A + B(S**X)          A =F10.5,11H        B =F10
   1.5,12H         X =F9.5,20H       SCALE FACTOR =F10.5)
600 FORMAT(1H0)
610 FORMAT(51H           (SIN()/L)**2          LOG K             W)
620 FORMAT(12H              F10.6,8H        F9.5,F13.0)
630 FORMAT(1H1,37H  U  V  W                 WEISSENBERG)
640 FORMAT(1H0,3I3,9H    LAYERI3,36H                            SCALE FACTOR
   1 =F10.5,26H      NO. OF REFLECTIONS =I5)
635 FORMAT(1H1,36H  U  V  W                 PRECESSION)
660 FORMAT(1H0,2H  3I4,F19.7,F18.6,F19.3,F18.4,3I10)
670 FORMAT(1H1,3I3,9H    LAYERI3)
650 FORMAT   (120H0     H   K   L              SIN()/L        LP FACTOR
   1             F**2                F              EPS         W
   2R )
680 FORMAT(5F9.2,F18.6,9H        R,12X)
690 FORMAT(1H0,49H          TOTAL NUMBER OF INDEPENDENT REFLECTIONSI7)
    END(2,2,2,2,2)
```

```
      SF NORM
      DIMENSION H1(1000),H2(1000),H3(1000),AVEQ(1000),EPS(1000),REJQ
     1(1000),RENO(1000),PL(1000),SI(1000),RAVEQ(1000),WEI(1000),Y1(50),
     2Y2(50),Y3(50),M1(1000),M2(1000),M3(1000),YAVEQ(50),YRAVEQ(50),
     3MRENO(1000),YWEI(50),MREJQ(1000),MEPS(1000), BS1(20),CS(20),
     4X(50,1),BCB(450),YSI(50),WI(100),AN(20),AS(20),AS1(20),BS(20)
      FREQUENCY 190(15),195(25),260(0,1,10),300(50,1,0),340(0,1,20),
     1362(5),363(300),390(0,1,10),435(0,3,1),205(5),    805(5,1,30),
     2480(2,1,15),364(5)
  180 REWIND 4
      READ INPUT TAPE 4,700
      READ TAPE 4,NASP
      READ TAPE 4,(AS(I),AS1(I),BS(I),BS1(I),CS(I),AN(I),I=1,NASP)
      READ TAPE 4,NOZ,NS,NI,BT1,BT2,SF,EX,NOIB,NRT
      REWIND 5
      REWIND 6
      REWIND 7
      REWIND 8
      WRITE OUTPUT TAPE 5,740,NOIB
      WRITE OUTPUT TAPE 7,740 ,NRT
      ON=1.0
      N=0
  185 AE2=0.0
      AE2C=0.0
      AE=0.0
      AEC=0.0
      AE21=0.0
      AE21C=0.0
  190 DO 330 J=1,NOZ
      READ TAPE 8,IBIG
      READ TAPE 8,(H1(I),H2(I),H3(I),AVEQ(I),EPS(I),REJQ(I),RENO(I),
     1SI(I),I=1,IBIG)
  195 DO 320 I=1,IBIG
      IF(AVEQ(I)-1.0E-10)220,220,200
  200 SIG=0.0
  205 DO 210 L=1,NASP
  210 SIG=SIG+AN(L)*(AS(L)*EXPF(-AS1(L)*SI(I))+BS(L)*EXPF(-BS1(L)*SI(I))
     1+CS(L))**2
      AVEQ(I)=AVEQ(I)*EXPF(BT1*(SI(I)**EX))/(EPS(I)*SIG)
  220 RAVEQ(I)=SQRTF(AVEQ(I))
      AVEQ(I)=AVEQ(I)-1.0
      AE=AE+RAVEQ(I)
      AEC=AEC+1.0
      AE21=AE21+AVEQ(I)
      AE21C=AE21C+1.0
      AE2=AE2+ABSF(AVEQ(I))
      AE2C=AE2C+1.0
      SI(I)=SQRTF(SI(I))
  260 IF(RENO(I))270,270,280
  270 WEI(I)=0.0
      GO TO 290
  280 WEI(I)=1.0/SQRTF(RENO(I))
  290 N=N+1
      Y1(N)=H1(I)
```

```
      Y2(N)=H2(I)
      Y3(N)=H3(I)
      M1(N)=INTG(H1(I))
      M2(N)=INTG(H2(I))
      M3(N)=INTG(H3(I))
      YSI(N)=SI(I)
      YAVEQ(N)=AVEQ(I)
      YRAVEQ(N)=RAVEQ(I)
      MRENO(N)=RENO(I)+.0001
      YWEI(N)=WEI(I)
      MREJQ(N)=REJQ(I)+.0001
      MEPS(N)=EPS(I)+.0001
  300 IF(N-25)320,310,310
  310 WRITE OUTPUT TAPE 9,540
      WRITE OUTPUT TAPE 9,600
      WRITE OUTPUT TAPE9,560,(M1(K),M2(K),M3(K),YSI(K),YAVEQ(K),YRAVEQ(K
     1),MEPS(K),MRENO(K),MREJQ(K),K=1,25)
      WRITE OUTPUT TAPE 5,680,(M1(K),M2(K),M3(K),YAVEQ(K),K=1,25)
      N=0
  320 CONTINUE
  330 CONTINUE
  340 IF(N)360,360,350
  350 WRITE OUTPUT TAPE 9,540
      WRITE OUTPUT TAPE 9,550
      WRITE OUTPUT TAPE9,560,(M1(K),M2(K),M3(K),YSI(K),YAVEQ(K),YRAVEQ(K
     1),MEPS(K),MRENO(K),MREJQ(K),K=1,N)
      WRITE OUTPUT TAPE 5,680,(M1(K),M2(K),M3(K),YAVEQ(K),K=1,N)
  360 END FILE 5
      REWIND 5
      REWIND 8
      WRITE OUTPUT TAPE 9,530
      WRITE OUTPUT TAPE 9,590,BT2,BT1,EX,SF
  361 ZAF=AF/AFC
      ZAF2=AF2/AF2C
      ZAF21=AF21/AF21C
      WRITE OUTPUT TAPE 9,600
      WRITE OUTPUT TAPE 9,690,ZAF,ZAE2,ZAE21
  362 DO 820 K=1,NS
      READ TAPE 6,U1,U2,U3,CE,PE
      READ TAPE 6,SL,NR,TL
      READ TAPE 6,(H1(J),H2(J),H3(J),EPS(J),AVEQ(J),REJQ(J),RENO(J),
     1PL(J),SI(J),J=1,NR)
      MU1=INTG(U1)
      MU2=INTG(U2)
      MU3=INTG(U3)
      MSL=INTG(SL)
  363 DO 430 I=1,NR
      SIG=0.0
  370 DO 380 L=1,NASP
  380 SIG=SIG+AN(L)*(AS(L)*EXPF(-AS1(L)*SI(I))+BS(L)*EXPF(-BS1(L)*SI(I))
     1+CS(L))**2
      PL(I)=EXPF(BT1*(SI(I)**EX))/(EPS(I)*SIG)
      IF(AVEQ(I)-1.0E-10)385,385,381
  381 AVEQ(I)=AVEQ(I)*PL(I)*SF
```

```
385 RAVEQ(I)=SQRTF(AVEQ(I))
    AVEQ(I)=AVEQ(I)-1.0
    SI(I)=SQRTF(SI(I))
390 IF(RENO(I))400,400,410
400 WEI(I)=0.0
    GO TO 420
410 WEI(I)=1.0/SQRTF(RENO(I))
420 M1(I)=INTG(H1(I))
    M2(I)=INTG(H2(I))
    M3(I)=INTG(H3(I))
429 MREJO(I)=REJO(I)+.0001
    MRENO(I)=RENO(I)+.0001
430 MEPS(I)=EPS(I)+.0001
    NR1=NR
435 IF(PF)437,437,436
436 WRITE OUTPUT TAPE 9,635
    GO TO 450
437 WRITE OUTPUT TAPE 9,630
450 WRITE OUTPUT TAPE 9,640,MU1,MU2,MU3,MSL,NR
470 WRITE OUTPUT TAPE 9,550
    WRITE OUTPUT TAPE 9,650
    WRITE OUTPUT TAPE 9,600
480 IF(NR1-22)490,490,800
490 NR2=NR-NR1+1
    WRITE OUTPUT TAPE 9,660,(M1(I),M2(I),M3(I),SI(I),PL(I),AVEQ(I),
   1RAVEQ(I),MEPS(I),MRENO(I),MREJO(I),I=NR2,NR)
    GO TO 810
800 NR2=NR-NR1+1
    NR3=NR2+23
    WRITE OUTPUT TAPE 9,660,(M1(I),M2(I),M3(I),SI(I),PL(I),AVEQ(I),
   1RAVEQ(I),MEPS(I),MRENO(I),MREJO(I),I=NR2,NR3)
    NR1=NR1-24
    WRITE OUTPUT TAPE 9,670,MU1,MU2,MU3,MSL
    WRITE OUTPUT TAPE 9,650
    WRITE OUTPUT TAPE 9,600
805 IF(NR1-24)490,490,800
810 WRITE OUTPUT TAPE 7,680,(M1(I),M2(I),M3(I),AVEQ(I),I=1,NR)
820 CONTINUE
    END FILE 7
    REWIND 6
    REWIND 7
    PRINT 730
    PAUSE
540 FORMAT(1H1,106H                H    K    L             SIN()/L
   1  E**2 - 1              E              EPS         W          R)
550 FORMAT(1H )
560 FORMAT(1H0,12H              3I4,F18.7,F19.5,F18.5,3I9)
530 FORMAT(1H1)
590 FORMAT(33H  LOG K = A + B(S**X)             A =F10.5,11H        B =F10
   1.5,12H          X =F9.5,20H       SCALE FACTOR =F10.5)
600 FORMAT(1H0)
630 FORMAT(1H1,37H  U   V   W                      WEISSENBERG)
640 FORMAT(1H0,3I3,9H     LAYERI3,36H                    NO. OF REFLECTIONS
   1 =I5)
```

```
635 FORMAT(1H1,36H  U  V  W                   PRECESSION)
660 FORMAT(1H0,2H  3I4,F19.7,F18.6,F19.5,F18.5,3I10)
670 FORMAT(1H1,3I3,9H    LAYERI3)
650 FORMAT   (120H0     H   K   L            SIN()/L            K
   1           E**2 - 1              E             EPS         W
   2R )
680 FORMAT(3I4,F20.5)
690 FORMAT(1H0,12H    AVE. E = F10.6,24H       AVE. /E**2 - 1/ =F10.6,
   122H       AVE. E**2 - 1 =F10.6)
700 FORMAT(72H
   1            )
710 FORMAT(I4,F5.4)
720 FORMAT(5F8.4,F4.0)
730 FORMAT(80H JOB FINISHED.  REMOVE AND SAVE TAPE 7.  USE TAPE 5 FOR
   1INPUT TO JOB E ORDERING. //////////// )
740 FORMAT(I7)
    END(0,1,0,0,1)
```

```
      E ORDER
      DIMENSION M1(2400),M2(2400),M3(2400),AV(2400),K1(2400),K2(2400),K
     1(2400),QAV(2400),R(2400)
      COMMON M1,M2,M3,AV,R
      FREQUENCY 5(5,1,5),30(1200),50(5,1,5),80(800),90(5,1,5),
     1170(1,1,5),180(25)
      REWIND 5
      READ INPUT TAPE 5,1001,NOIB
    1 IF(5000-NOIB)2,3,3
    2 NIBO=5000
      NOIB=NOIB-5000
      NBIO=1
      GO TO 4
    3 NBIO=2
      NIBO=NOIB
    4 K=0
      L=0
      DO 20 I=1,NIBO
      READ INPUT TAPE 5,1000,N1,N2,N3,Q
    5 IF(Q)20,10,10
   10 L=L+1
      M1(L)=N1
      M2(L)=N2
      M3(L)=N3
      AV(L)=Q
   20 CONTINUE
   30 DO 160 J=1,L
   40 DO 70 K=1,L
   50 IF(AV(K))70,60,60
   60 BAV=AV(K)
      GO TO 80
   70 CONTINUE
   80 DO 110 I=K,L
   90 IF(AV(I)-BAV)110,100,100
  100 BAV=AV(I)
      I1=I
  110 CONTINUE
      K1(J)=M1(I1)
      K2(J)=M2(I1)
      K3(J)=M3(I1)
      QAV(J)=AV(I1)
      R(J)=SQRTF(AV(I1)+1.0)
      AV(I1)=-1.0
  160 CONTINUE
      WRITE OUTPUT TAPE 9,1006
      WRITE OUTPUT TAPE 9,1001,NOIB
      M=L/50
  170 IF(M-1)200,180,180
  180 DO 190 I=1,M
      N=I*50-49
      N1=N+24
      WRITE OUTPUT TAPE 9,1002
      WRITE OUTPUT TAPE 9,1003
  190 WRITE OUTPUT TAPE 9,1004,(K1(J),K2(J),K3(J),QAV(J),R(J),K1(J+25),
```

```
     1K2(J+25),K3(J+25),QAV(J+25),R(J+25),J=N,N1)
 200 WRITE OUTPUT TAPE 9,1002
     WRITE OUTPUT TAPE 9,1003
     L1=L-50*M
     L2=L1-25
     IF(L2)220,220,210
 210 N=M*50+1
     N1=N+L2-1
     WRITE OUTPUT TAPE 9,1004,(K1(J),K2(J),K3(J),QAV(J),R(J),K1(J+25),
     1K2(J+25),K3(J+25),QAV(J+25),R(J+25),J=N,N1)
     N2=N1+1
     N3=N+24
     WRITE OUTPUT TAPE 9,1005,(K1(J),K2(J),K3(J),QAV(J),R(J),J=N2,N3)
     GO TO 230
 220 N=M*50+1
     N1=M*50+L1
     WRITE OUTPUT TAPE 9,1005,(K1(J),K2(J),K3(J),QAV(J),R(J),J=N,N1)
 230 CALL OUI(K1,K2,K3,QAV,L)
     GO TO(1,240),NBIO
 240 PRINT 1007
     STOP
1000 FORMAT(3I4,F20.5)
1001 FORMAT(I7)
1002 FORMAT(1H1,107H            H    K    L         E**2 - 1          E
    1                     H    K    L         E**2 - 1          E)
1003 FORMAT(1H0)
1004 FORMAT(1H0,I13,2I4,2F15.5,I22,2I4,2F15.5)
1005 FORMAT(1H0,I13,2I4,2F15.5)
1006 FORMAT(1H1)
1007 FORMAT(1H1,28H JOB FINISHED.  SAVE TAPE 5./////)
     END(1,1,0,0,1)
```

```
      SUBROUTINE OUI(K1,K2,K3,QAV,L)
      DIMENSION K1(2400),K2(2400),K3(2400),QAV(2400),KU(300,8),LU(300,
     18),MU(300,8),Q(300,8) ,S(300,8)
      COMMON KU,LU,MU,Q ,S
      J1=0
      J2=0
      J3=0
      J4=0
      J5=0
      J6=0
      J7=0
      J8=0
   10 DO 300 J=1,L
   20 IF(K1(J)-K1(J)/2-K1(J)/2)40,30,40
   30 I1=2
      GO TO 50
   40 I1=1
   50 IF(K2(J)-K2(J)/2-K2(J)/2)70,60,70
   60 I2=2
      GO TO 80
   70 I2=1
   80 IF(K3(J)-K3(J)/2-K3(J)/2)95,90,95
   90 I3=2
      GO TO 99
   95 I3=1
   99 GO TO(100,200),I1
  100 GO TO(110,120),I2
  110 GO TO(111,112),I3
  120 GO TO(121,122),I3
  200 GO TO(210,220),I2
  210 GO TO(211,212),I3
  220 GO TO(221,222),I3
  111 J8=J8+1
      KU(J8,8)=K1(J)
      LU(J8,8)=K2(J)
      MU(J8,8)=K3(J)
      Q(J8,8)=QAV(J)
      S(J8,8)=SQRTF(QAV(J)+1.0)
      GO TO 300
  112 J5=J5+1
      KU(J5,5)=K1(J)
      LU(J5,5)=K2(J)
      MU(J5,5)=K3(J)
      Q(J5,5)=QAV(J)
      S(J5,5)=SQRTF(QAV(J)+1.0)
      GO TO 300
  121 J6=J6+1
      Q(J6,6)=QAV(J)
      KU(J6,6)=K1(J)
      LU(J6,6)=K2(J)
      MU(J6,6)=K3(J)
      S(J6,6)=SQRTF(QAV(J)+1.0)
      GO TO 300
  122 J2=J2+1
```

```
      KU(J2,2)=K1(J)
      LU(J2,2)=K2(J)
      MU(J2,2)=K3(J)
      Q(J2,2)=QAV(J)
      S(J2,2)=SQRTF(QAV(J)+1.0)
      GO TO 300
  211 J7=J7+1
      KU(J7,7)=K1(J)
      LU(J7,7)=K2(J)
      MU(J7,7)=K3(J)
      Q(J7,7)=QAV(J)
      S(J7,7)=SQRTF(QAV(J)+1.0)
      GO TO 300
  212 J3=J3+1
      KU(J3,3)=K1(J)
      LU(J3,3)=K2(J)
      MU(J3,3)=K3(J)
      Q(J3,3)=QAV(J)
      S(J3,3)=SQRTF(QAV(J)+1.0)
      GO TO 300
  221 J4=J4+1
      KU(J4,4)=K1(J)
      LU(J4,4)=K2(J)
      MU(J4,4)=K3(J)
      Q(J4,4)=QAV(J)
      S(J4,4)=SQRTF(QAV(J)+1.0)
      GO TO 300
  222 J1=J1+1
      KU(J1,1)=K1(J)
      LU(J1,1)=K2(J)
      MU(J1,1)=K3(J)
      Q(J1,1)=QAV(J)
      S(J1,1)=SQRTF(QAV(J)+1.0)
  300 CONTINUE
      LL=J1
      DO 500 K=1,8
      M=LL/50
  310 IF(M-1)340,320,320
  320 DO 330 I=1,M
      N=I*50-49
      N1=N+24
      WRITE OUTPUT TAPE 9,1002
      WRITE OUTPUT TAPE 9,1003
  330 WRITE OUTPUT TAPE 9,1004,(KU(J,K),LU(J,K),MU(J,K),Q(J,K),S(J,K),
     1KU(J+25,K),LU(J+25,K),MU(J+25,K),Q(J+25,K),S(J+25,K),J=N,N1)
  340 WRITE OUTPUT TAPE 9,1002
      WRITE OUTPUT TAPE 9,1003
      L1=LL-50*M
      L2=L1-25
  350 IF(L2)370,370,360
  360 N=M*50+1
      N1=N+L2-1
      WRITE OUTPUT TAPE 9,1004,(KU(J,K),LU(J,K),MU(J,K),Q(J,K),S(J,K),
     1KU(J+25,K),LU(J+25,K),MU(J+25,K),Q(J+25,K),S(J+25,K),J=N,N1)
```

```
      N2=N1+1
      N3=N+24
      WRITE OUTPUT TAPE 9,1005,(KU(J,K),LU(J,K),MU(J,K),Q(J,K),S(J,K),
     1J=N2,N3)
      GO TO 380
  370 N=M*50+1
      N1=M*50+L1
      WRITE OUTPUT TAPE 9,1005,(KU(J,K),LU(J,K),MU(J,K),Q(J,K),S(J,K),
     1J=N,N1)
  380 GO TO(390,400,410,420,430,440,450,500),K
  390 LL=J2
      GO TO 500
  400 LL=J3
      GO TO 500
  410 LL=J4
      GO TO 500
  420 LL=J5
      GO TO 500
  430 LL=J6
      GO TO 500
  440 LL=J7
      GO TO 500
  450 LL=J8
  500 CONTINUE
      RETURN
 1002 FORMAT(1H1,107H            H    K    L          E**2 - 1           E
     1                H    K    L          E**2 - 1           E)
 1003 FORMAT(1H0)
 1004 FORMAT(1H0,I13,2I4,2F15.5,I22,2I4,2F15.5)
 1005 FORMAT(1H0,I13,2I4,2F15.5)
      END(2,2,2,2,2)
```

```
   FUNCTION INTG(A)
   IF(A)20,10,20
10 INTG=0
   GO TO 30
20 INTG=XSIGNF(XINTF(ABSF(A)+.1),XINTF(A))
30 RETURN
   END(2,2,2,2,2)
```

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Naval Research Laboratory. Report 5739. AN X-RAY DIFFRACTION DATA REDUCTION PROGRAM FOR THE IBM 704 AND 7090, by H. G. Norment. 62 pp. and figs., February 16, 1962.

This program is intended to provide a completely automatic process for reducing "raw" single-crystal x-ray diffraction intensity data to the form of structure factors. If desired, the data reduction may be extended to yield normalized structure factors. The program is applicable primarily to data obtained on film with Weissenberg and/or precession goniometers.

All programming has been done in IBM 704 FORTRAN II language. Binary program decks are available which are independent of any special operating system.

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